



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:55 PM UTC

PDB ID : 6RZ5 / pdb_00006rz5
Title : XFEL crystal structure of the human cysteinyl leukotriene receptor 1 in complex with zafirlukast
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Deposited on : 2019-06-12
Resolution : 2.53 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12

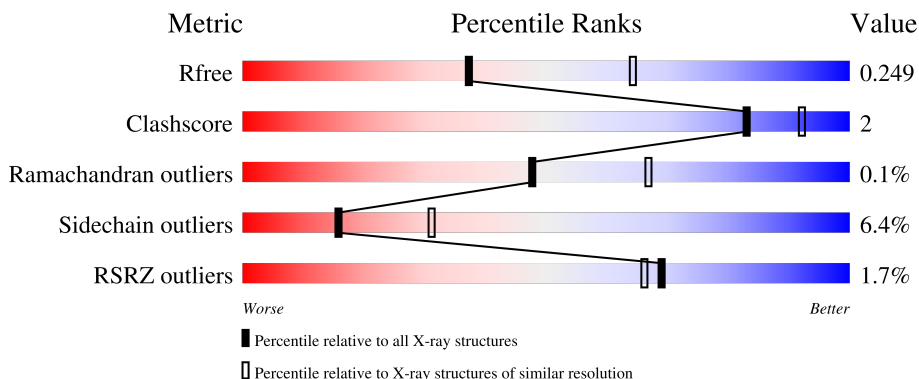
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

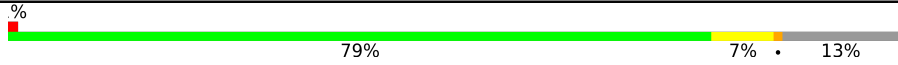
The reported resolution of this entry is 2.53 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	423	
1	B	423	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.49

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OLC	B	2010	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6138 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

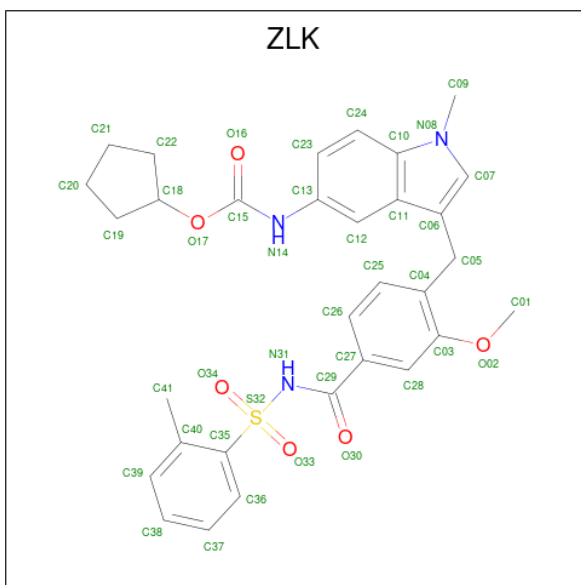
- Molecule 1 is a protein called Cysteinyl leukotriene receptor 1, Soluble cytochrome b562, Cysteinyl leukotriene receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	1	0
			2719	1781	437	477	24			
1	B	385	Total	C	N	O	S	0	2	0
			2837	1851	462	499	25			

There are 18 discrepancies between the modelled and reference sequences:

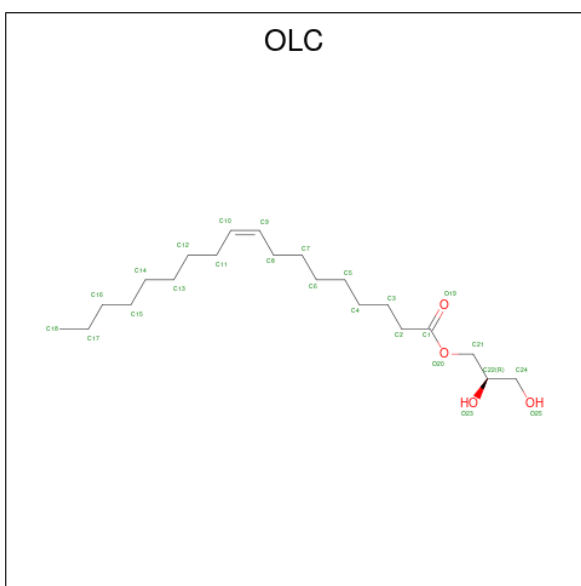
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9Y271
A	-1	GLY	-	expression tag	UNP Q9Y271
A	0	THR	-	expression tag	UNP Q9Y271
A	1000	SER	-	linker	UNP Q9Y271
A	1007	TRP	MET	conflict	UNP P0ABE7
A	1102	ILE	HIS	conflict	UNP P0ABE7
A	1106	LEU	-	linker	UNP P0ABE7
A	?	SER	-	linker	UNP P0ABE7
A	?	GLY	-	linker	UNP P0ABE7
B	-2	GLY	-	expression tag	UNP Q9Y271
B	-1	GLY	-	expression tag	UNP Q9Y271
B	0	THR	-	expression tag	UNP Q9Y271
B	1000	SER	-	linker	UNP Q9Y271
B	1007	TRP	MET	conflict	UNP P0ABE7
B	1102	ILE	HIS	conflict	UNP P0ABE7
B	1106	LEU	-	linker	UNP P0ABE7
B	?	SER	-	linker	UNP P0ABE7
B	?	GLY	-	linker	UNP P0ABE7

- Molecule 2 is zafirlukast (CCD ID: ZLK) (formula: C₃₁H₃₃N₃O₆S) (labeled as "Ligand of Interest" by depositor).



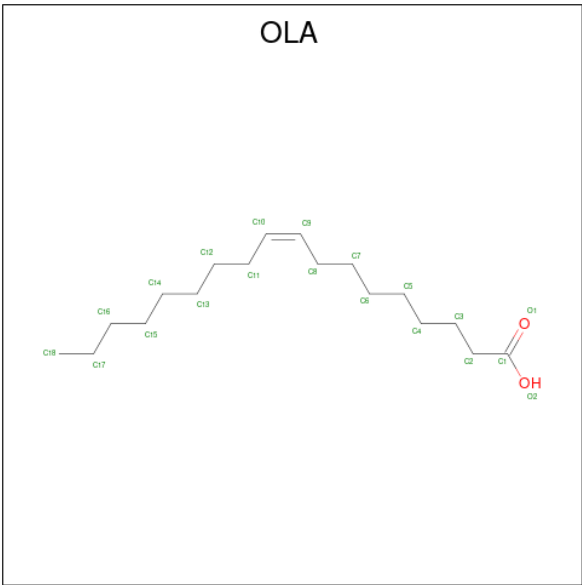
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			41	31	3	6	1		
2	B	1	Total	C	N	O	S	0	0
			41	31	3	6	1		
2	B	1	Total	C	N	O	S	0	0
			41	31	3	6	1		

- Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 9 9	0	0
3	A	1	Total C 17 17	0	0
3	A	1	Total C 11 11	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 12 12	0	0
3	A	1	Total C O 16 12 4	0	0
3	A	1	Total C 9 9	0	0
3	A	1	Total C 7 7	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 9 9	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 7 7	0	0
3	B	1	Total C O 23 19 4	0	0
3	B	1	Total C O 7 5 2	0	0

- Molecule 4 is OLEIC ACID (CCD ID: OLA) (formula: C₁₈H₃₄O₂).



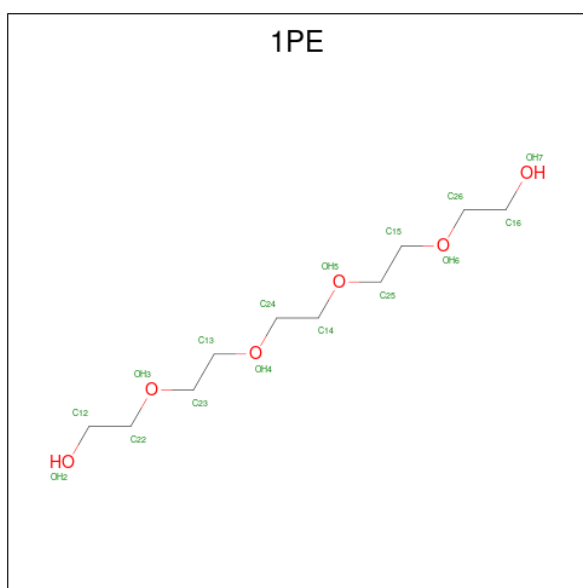
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	9	2		
4	A	1	Total	C	O	0	0
			13	11	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			19	17	2		
4	A	1	Total	C	O	0	0
			7	5	2		
4	A	1	Total	C	O	0	0
			7	5	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			13	11	2		
4	A	1	Total	C		0	0
			6	6			
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			14	12	2		
4	B	1	Total	C	O	0	0
			12	10	2		
4	B	1	Total	C	O	0	0
			10	8	2		
4	B	1	Total	C	O	0	0
			16	14	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			9	7	2		
4	B	1	Total	C	O	0	0
			11	9	2		
4	B	1	Total	C	O	0	0
			20	18	2		
4	B	1	Total	C	O	0	0
			18	16	2		
4	B	1	Total	C	O	0	0
			20	18	2		

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	B	1	Total	Na	0	0
			1	1		

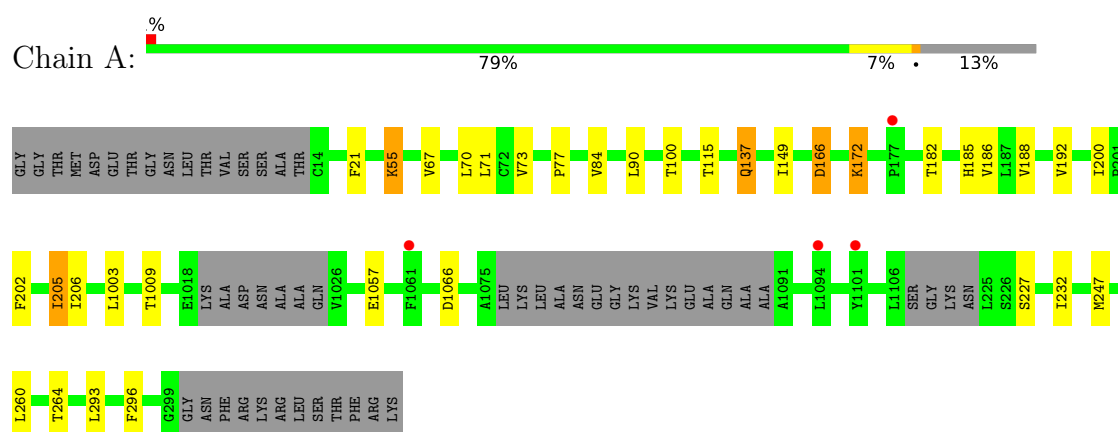
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total 5	O 5	0	0
7	B	5	Total 5	O 5	0	0

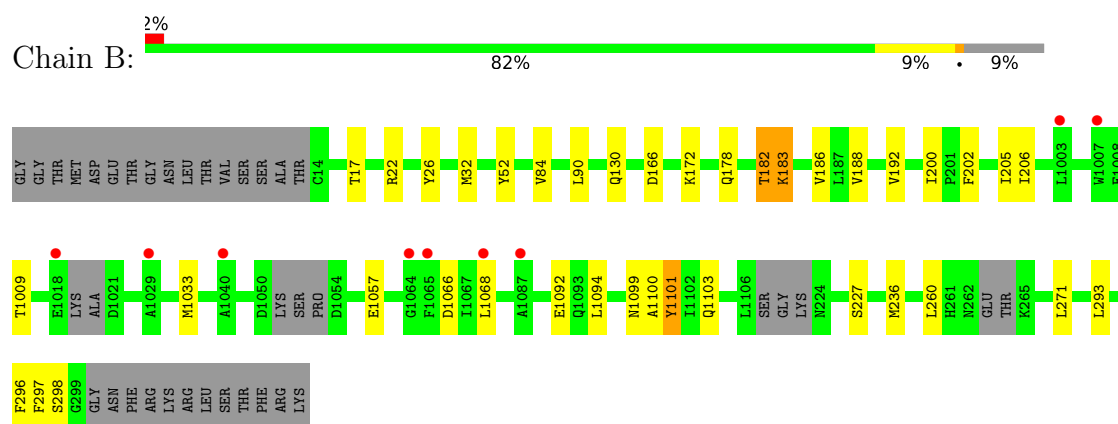
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cysteinyl leukotriene receptor 1, Soluble cytochrome b562, Cysteinyl leukotriene receptor 1



- Molecule 1: Cysteinyl leukotriene receptor 1, Soluble cytochrome b562, Cysteinyl leukotriene receptor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.59Å 68.58Å 87.39Å 76.31° 76.68° 81.21°	Depositor
Resolution (Å)	19.84 – 2.53 19.84 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.84-2.53) 99.5 (19.84-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.53Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.189 , 0.223 0.216 , 0.249	Depositor DCC
R_{free} test set	1514 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 135.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6138	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLA, 1PE, OLC, NA, ZLK

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.91	0/2784	1.49	10/3807 (0.3%)
1	B	0.92	2/2901 (0.1%)	1.48	6/3960 (0.2%)
All	All	0.91	2/5685 (0.0%)	1.49	16/7767 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	32	MET	SD-CE	-5.52	1.65	1.79
1	B	200	ILE	CA-CB	5.29	1.57	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	PHE	CA-CB-CG	8.53	122.33	113.80
1	B	200	ILE	N-CA-CB	7.07	115.97	110.45
1	A	200	ILE	N-CA-CB	6.92	115.85	110.45
1	A	166	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	21	PHE	CA-C-N	5.86	128.06	120.44
1	A	21	PHE	C-N-CA	5.86	128.06	120.44
1	A	186	VAL	N-CA-C	-5.47	104.11	111.44
1	B	52	TYR	CA-C-N	5.41	127.84	120.54
1	B	52	TYR	C-N-CA	5.41	127.84	120.54
1	B	227	SER	CA-C-N	5.39	129.80	120.58
1	B	227	SER	C-N-CA	5.39	129.80	120.58
1	A	100	THR	CA-C-N	5.26	127.27	120.44
1	A	100	THR	C-N-CA	5.26	127.27	120.44
1	A	227	SER	CA-C-N	5.25	129.56	120.58
1	A	227	SER	C-N-CA	5.25	129.56	120.58
1	B	1100	ALA	N-CA-C	5.10	116.64	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2719	0	2514	13	0
1	B	2837	0	2602	11	0
2	A	41	0	0	0	0
2	B	82	0	0	0	0
3	A	89	0	130	0	0
3	B	94	0	129	2	0
4	A	138	0	184	6	0
4	B	116	0	165	3	0
5	A	10	0	13	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
All	All	6138	0	5737	28	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (28) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185[A]:HIS:HB2	4:A:2014:OLA:H32	1.68	0.76
1:A:55:LYS:O	1:A:137:GLN:HG2	1.92	0.70
1:B:182:THR:HG21	1:B:260:LEU:HD13	1.80	0.63
1:B:1099:ASN:HA	1:B:1103:GLN:HB2	1.83	0.60
1:B:296:PHE:HB3	4:B:2013:OLA:H41	1.84	0.59
3:B:2004:OLC:H6A	3:B:2006:OLC:H11	1.89	0.54
1:A:185[B]:HIS:HB2	4:A:2014:OLA:H32	1.88	0.54
1:A:67:VAL:HG11	4:A:2013:OLA:H62	1.92	0.51
1:B:1101:TYR:N	1:B:1101:TYR:CD2	2.79	0.51
1:B:293:LEU:HD22	1:B:297:PHE:HE2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ILE:HD11	4:A:2012:OLA:H42	1.92	0.50
1:A:70:LEU:HA	1:A:73:VAL:HG22	1.93	0.49
1:A:166:ASP:HB3	1:A:172:LYS:HD2	1.94	0.49
1:A:202:PHE:HE2	1:A:247:MET:HE2	1.79	0.48
1:B:22:ARG:O	1:B:26:TYR:HB2	2.14	0.47
4:A:2019:OLA:H10	4:B:2016:OLA:H182	1.96	0.46
4:B:2011:OLA:H32	4:B:2014:OLA:H31	1.97	0.46
4:A:2019:OLA:H41	3:B:2010:OLC:H3A	1.99	0.44
1:B:188:VAL:O	1:B:192:VAL:HG23	2.18	0.44
1:A:202:PHE:CE2	1:A:247:MET:HE2	2.52	0.43
1:B:1033:MET:HE1	1:B:1094:LEU:HD13	2.00	0.43
1:A:115:THR:HA	1:A:205:ILE:HD11	2.01	0.43
1:A:73:VAL:O	1:A:77:PRO:HD3	2.19	0.42
1:B:202:PHE:O	1:B:206:ILE:HG12	2.20	0.41
1:A:188:VAL:O	1:A:192:VAL:HG23	2.19	0.41
1:B:166:ASP:HB3	1:B:172:LYS:HE3	2.02	0.41
1:A:202:PHE:O	1:A:206:ILE:HG12	2.20	0.41
1:B:182:THR:CG2	1:B:260:LEU:HD13	2.50	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	362/423 (86%)	350 (97%)	12 (3%)	0	100	100
1	B	377/423 (89%)	368 (98%)	8 (2%)	1 (0%)	36	53
All	All	739/846 (87%)	718 (97%)	20 (3%)	1 (0%)	48	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	183	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/375 (71%)	249 (94%)	16 (6%)	17	34
1	B	269/375 (72%)	251 (93%)	18 (7%)	15	29
All	All	534/750 (71%)	500 (94%)	34 (6%)	16	31

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	71	LEU
1	A	84	VAL
1	A	90	LEU
1	A	137	GLN
1	A	149	ILE
1	A	172	LYS
1	A	182	THR
1	A	205	ILE
1	A	1003	LEU
1	A	1009	THR
1	A	1057	GLU
1	A	1066	ASP
1	A	260	LEU
1	A	264	THR
1	A	293	LEU
1	B	17	THR
1	B	84	VAL
1	B	90	LEU
1	B	130	GLN
1	B	178	GLN
1	B	182	THR
1	B	183	LYS

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Mol	Chain	Res	Type
1	B	186	VAL
1	B	205	ILE
1	B	1009	THR
1	B	1057	GLU
1	B	1066	ASP
1	B	1068	LEU
1	B	1092	GLU
1	B	1101	TYR
1	B	236	MET
1	B	271	LEU
1	B	298	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	41	ASN
1	A	137	GLN
1	A	170	ASN
1	A	184	ASN
1	B	130	GLN
1	B	170	ASN
1	B	184	ASN
1	B	1025	GLN
1	B	1099	ASN
1	B	1103	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 42 ligands modelled in this entry, 2 are monoatomic - leaving 40 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ZLK	B	2001	-	45,45,45	2.41	20 (44%)	64,65,65	2.49	22 (34%)
4	OLA	A	2017	-	12,12,19	0.65	0	12,12,19	0.85	0
3	OLC	A	2002	-	8,8,24	0.42	0	7,7,25	0.58	0
3	OLC	A	2003	-	16,16,24	0.44	0	15,15,25	0.59	0
5	1PE	A	2021	-	9,9,15	0.49	0	8,8,14	0.22	0
4	OLA	B	2015	-	10,10,19	0.67	0	10,10,19	0.92	0
4	OLA	A	2018	-	5,5,19	0.46	0	4,4,19	0.66	0
3	OLC	A	2004	-	10,10,24	0.42	0	9,9,25	0.50	0
3	OLC	A	2007	-	15,15,24	0.75	0	16,16,25	1.02	1 (6%)
3	OLC	B	2009	-	22,22,24	0.68	1 (4%)	23,23,25	1.07	1 (4%)
4	OLA	B	2018	-	19,19,19	0.54	0	19,19,19	0.66	0
4	OLA	A	2010	-	10,10,19	0.69	0	10,10,19	0.75	0
4	OLA	A	2016	-	19,19,19	0.50	0	19,19,19	0.85	0
3	OLC	B	2010	-	6,6,24	2.49	2 (33%)	6,6,25	1.34	1 (16%)
4	OLA	B	2017	-	17,17,19	0.56	0	17,17,19	0.76	0
4	OLA	A	2012	-	7,7,19	0.78	0	7,7,19	0.96	0
4	OLA	A	2015	-	6,6,19	0.86	0	6,6,19	1.09	0
3	OLC	B	2002	-	7,7,24	0.39	0	6,6,25	0.63	0
2	ZLK	B	2019	-	45,45,45	2.30	24 (53%)	64,65,65	2.50	15 (23%)
4	OLA	B	2013	-	15,15,19	0.59	0	15,15,19	0.61	0
2	ZLK	A	2001	-	45,45,45	2.33	24 (53%)	64,65,65	2.47	20 (31%)
3	OLC	A	2005	-	7,7,24	0.46	0	6,6,25	0.46	0
4	OLA	B	2012	-	9,9,19	0.74	0	9,9,19	0.79	0
4	OLA	A	2011	-	12,12,19	0.67	0	12,12,19	0.69	0
4	OLA	A	2014	-	6,6,19	0.83	0	6,6,19	0.95	0
3	OLC	A	2009	-	6,6,24	0.31	0	5,5,25	0.68	0
4	OLA	A	2020	-	13,13,19	0.69	0	13,13,19	0.54	0
3	OLC	B	2008	-	6,6,24	0.35	0	5,5,25	0.75	0
4	OLA	B	2016	-	19,19,19	0.53	0	19,19,19	0.70	0
4	OLA	A	2019	-	19,19,19	0.52	0	19,19,19	0.66	0
4	OLA	B	2011	-	11,11,19	0.71	0	11,11,19	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OLC	A	2006	-	11,11,24	0.46	0	10,10,25	0.66	0
4	OLA	A	2013	-	18,18,19	0.60	0	18,18,19	0.60	0
3	OLC	B	2003	-	8,8,24	0.54	0	7,7,25	0.62	0
4	OLA	B	2014	-	8,8,19	0.74	0	8,8,19	0.93	0
3	OLC	B	2005	-	9,9,24	0.45	0	8,8,25	0.51	0
3	OLC	B	2004	-	9,9,24	0.42	0	8,8,25	0.65	0
3	OLC	A	2008	-	8,8,24	0.45	0	7,7,25	0.49	0
3	OLC	B	2007	-	9,9,24	0.49	0	8,8,25	0.49	0
3	OLC	B	2006	-	9,9,24	0.47	0	8,8,25	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ZLK	B	2001	-	-	2/29/36/36	0/5/5/5
4	OLA	A	2017	-	-	7/10/10/17	-
3	OLC	A	2002	-	-	4/6/6/24	-
3	OLC	A	2003	-	-	9/14/14/24	-
5	1PE	A	2021	-	-	4/7/7/13	-
4	OLA	B	2015	-	-	5/8/8/17	-
4	OLA	A	2018	-	-	2/3/3/17	-
3	OLC	A	2004	-	-	2/8/8/24	-
3	OLC	A	2007	-	-	11/15/15/24	-
3	OLC	B	2009	-	-	13/22/22/24	-
4	OLA	B	2018	-	-	12/17/17/17	-
4	OLA	A	2010	-	-	5/8/8/17	-
4	OLA	A	2016	-	-	11/17/17/17	-
3	OLC	B	2010	-	-	4/4/4/24	-
4	OLA	B	2017	-	-	10/15/15/17	-
4	OLA	A	2012	-	-	5/5/5/17	-
4	OLA	A	2015	-	-	2/4/4/17	-
3	OLC	B	2002	-	-	1/5/5/24	-
2	ZLK	B	2019	-	-	8/29/36/36	0/5/5/5
4	OLA	B	2013	-	-	10/13/13/17	-
2	ZLK	A	2001	-	-	2/29/36/36	0/5/5/5
3	OLC	A	2005	-	-	2/5/5/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLA	B	2012	-	-	6/7/7/17	-
4	OLA	A	2011	-	-	6/10/10/17	-
4	OLA	A	2014	-	-	3/4/4/17	-
3	OLC	A	2009	-	-	4/4/4/24	-
4	OLA	A	2020	-	-	3/11/11/17	-
3	OLC	B	2008	-	-	2/4/4/24	-
4	OLA	B	2016	-	-	7/17/17/17	-
4	OLA	A	2019	-	-	12/17/17/17	-
4	OLA	B	2011	-	-	4/9/9/17	-
3	OLC	A	2006	-	-	5/9/9/24	-
4	OLA	A	2013	-	-	11/16/16/17	-
3	OLC	B	2003	-	-	3/6/6/24	-
4	OLA	B	2014	-	-	5/6/6/17	-
3	OLC	B	2005	-	-	4/7/7/24	-
3	OLC	B	2004	-	-	5/7/7/24	-
3	OLC	A	2008	-	-	3/6/6/24	-
3	OLC	B	2007	-	-	4/7/7/24	-
3	OLC	B	2006	-	-	3/7/7/24	-

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	ZLK	C29-N31	5.67	1.45	1.39
2	B	2001	ZLK	C15-N14	5.62	1.47	1.36
2	A	2001	ZLK	C15-N14	5.44	1.47	1.36
2	B	2019	ZLK	C15-N14	4.89	1.45	1.36
2	A	2001	ZLK	C29-N31	4.74	1.44	1.39
3	B	2010	OLC	O19-C1	4.73	1.37	1.22
2	B	2019	ZLK	C05-C04	4.72	1.58	1.51
2	B	2001	ZLK	O17-C15	4.37	1.43	1.35
2	B	2019	ZLK	C29-N31	4.32	1.44	1.39
2	A	2001	ZLK	O17-C15	3.91	1.42	1.35
2	A	2001	ZLK	C05-C04	3.76	1.56	1.51
2	B	2019	ZLK	O17-C15	3.70	1.41	1.35
2	B	2019	ZLK	C20-C19	-3.60	1.37	1.51
2	B	2001	ZLK	C20-C19	-3.58	1.37	1.51
3	B	2010	OLC	O20-C1	-3.54	1.19	1.30
2	A	2001	ZLK	C03-C04	3.51	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	ZLK	C20-C19	-3.42	1.38	1.51
2	B	2019	ZLK	C41-C40	3.34	1.57	1.51
2	A	2001	ZLK	C41-C40	3.32	1.57	1.51
2	B	2001	ZLK	C41-C40	3.30	1.57	1.51
2	B	2019	ZLK	O33-S32	3.23	1.47	1.43
2	B	2001	ZLK	C13-N14	3.22	1.48	1.41
2	B	2001	ZLK	C35-S32	3.12	1.81	1.77
2	B	2001	ZLK	C26-C25	3.05	1.43	1.38
2	B	2019	ZLK	C19-C18	2.98	1.66	1.52
2	A	2001	ZLK	C19-C18	2.98	1.66	1.52
2	B	2001	ZLK	C05-C04	2.97	1.55	1.51
2	B	2001	ZLK	C19-C18	2.96	1.66	1.52
2	B	2019	ZLK	C26-C25	2.93	1.43	1.38
2	A	2001	ZLK	C27-C29	2.86	1.56	1.50
2	A	2001	ZLK	C22-C18	-2.84	1.37	1.52
2	B	2001	ZLK	C22-C18	-2.83	1.37	1.52
2	A	2001	ZLK	C26-C25	2.80	1.43	1.38
2	B	2019	ZLK	C27-C29	2.79	1.56	1.50
2	B	2001	ZLK	C03-C04	2.76	1.44	1.39
2	B	2019	ZLK	C13-N14	2.75	1.47	1.41
2	B	2019	ZLK	C22-C18	-2.75	1.38	1.52
2	B	2001	ZLK	C27-C29	2.69	1.56	1.50
2	A	2001	ZLK	O02-C03	2.68	1.41	1.37
2	B	2001	ZLK	C26-C27	2.68	1.43	1.39
2	B	2001	ZLK	C12-C11	2.67	1.44	1.39
2	B	2019	ZLK	C12-C11	2.62	1.43	1.39
2	B	2001	ZLK	S32-N31	2.60	1.70	1.64
2	B	2001	ZLK	C28-C03	2.51	1.43	1.38
2	B	2001	ZLK	O02-C03	2.48	1.41	1.37
2	B	2001	ZLK	O33-S32	2.40	1.46	1.43
2	B	2019	ZLK	C28-C03	2.38	1.42	1.38
2	A	2001	ZLK	O30-C29	-2.35	1.17	1.23
2	A	2001	ZLK	C28-C03	2.34	1.42	1.38
2	A	2001	ZLK	S32-N31	2.34	1.69	1.64
2	A	2001	ZLK	C26-C27	2.29	1.42	1.39
2	B	2019	ZLK	O30-C29	-2.27	1.18	1.23
2	A	2001	ZLK	C12-C11	2.27	1.43	1.39
2	A	2001	ZLK	O34-S32	2.26	1.46	1.43
2	A	2001	ZLK	C21-C22	2.25	1.61	1.51
3	B	2009	OLC	O20-C1	2.25	1.39	1.33
2	B	2019	ZLK	C26-C27	2.23	1.42	1.39
2	A	2001	ZLK	O33-S32	2.20	1.46	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2019	ZLK	O16-C15	-2.19	1.17	1.21
2	A	2001	ZLK	O17-C18	-2.16	1.41	1.46
2	B	2019	ZLK	C23-C13	2.13	1.42	1.39
2	B	2019	ZLK	S32-N31	2.13	1.69	1.64
2	B	2019	ZLK	O34-S32	2.11	1.46	1.43
2	A	2001	ZLK	C35-S32	2.11	1.80	1.77
2	A	2001	ZLK	C24-C10	2.11	1.42	1.39
2	B	2019	ZLK	C35-S32	2.08	1.80	1.77
2	B	2019	ZLK	C24-C10	2.07	1.42	1.39
2	B	2019	ZLK	C25-C04	2.06	1.43	1.39
2	B	2001	ZLK	C21-C22	2.04	1.60	1.51
2	A	2001	ZLK	C13-N14	2.03	1.45	1.41
2	B	2019	ZLK	C21-C22	2.03	1.60	1.51

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	ZLK	O34-S32-O33	-13.55	103.06	119.52
2	B	2019	ZLK	O34-S32-O33	-12.39	104.47	119.52
2	B	2001	ZLK	O34-S32-O33	-12.03	104.91	119.52
2	B	2019	ZLK	O17-C15-N14	8.09	118.92	108.97
2	B	2001	ZLK	O17-C15-N14	6.76	117.28	108.97
2	B	2001	ZLK	C29-N31-S32	-5.53	116.12	123.38
2	B	2019	ZLK	C29-N31-S32	-5.46	116.22	123.38
2	A	2001	ZLK	O17-C15-N14	4.68	114.72	108.97
2	A	2001	ZLK	O02-C03-C04	4.49	122.64	115.96
2	A	2001	ZLK	C06-C07-N08	-4.11	107.22	110.55
2	A	2001	ZLK	O34-S32-C35	3.90	114.13	107.68
2	B	2001	ZLK	C06-C07-N08	-3.90	107.39	110.55
2	B	2019	ZLK	O02-C03-C04	3.78	121.59	115.96
2	B	2001	ZLK	O02-C03-C04	3.74	121.52	115.96
2	B	2019	ZLK	C06-C07-N08	-3.42	107.78	110.55
2	B	2019	ZLK	C18-O17-C15	3.22	121.12	116.52
2	B	2019	ZLK	O16-C15-N14	-3.20	119.32	126.12
2	B	2001	ZLK	C25-C04-C03	3.19	122.74	118.37
2	A	2001	ZLK	C29-N31-S32	-3.18	119.20	123.38
2	B	2019	ZLK	O33-S32-C35	3.12	112.83	107.68
2	B	2001	ZLK	C27-C29-N31	3.10	119.78	116.08
3	B	2009	OLC	O20-C1-C2	3.05	121.14	111.83
2	A	2001	ZLK	C39-C40-C35	3.01	119.45	116.27
2	B	2019	ZLK	O34-S32-C35	3.00	112.64	107.68
2	B	2001	ZLK	C39-C40-C35	2.99	119.42	116.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2019	ZLK	C39-C40-C35	2.91	119.34	116.27
2	B	2019	ZLK	O02-C03-C28	-2.85	119.17	124.08
2	B	2001	ZLK	O16-C15-N14	-2.83	120.10	126.12
2	B	2001	ZLK	C35-S32-N31	2.83	109.47	105.96
2	A	2001	ZLK	C05-C04-C25	-2.80	115.48	120.06
2	A	2001	ZLK	C10-N08-C07	2.77	110.55	108.54
3	A	2007	OLC	O20-C1-C2	2.75	120.22	111.83
2	A	2001	ZLK	C25-C04-C03	2.73	122.11	118.37
2	A	2001	ZLK	O02-C03-C28	-2.73	119.37	124.08
2	A	2001	ZLK	C01-O02-C03	2.68	121.44	117.51
2	B	2001	ZLK	C11-C06-C07	2.65	108.75	106.34
2	B	2001	ZLK	C26-C25-C04	-2.53	118.08	121.39
2	B	2001	ZLK	C28-C03-C04	-2.51	117.90	120.49
2	A	2001	ZLK	C35-S32-N31	2.47	109.03	105.96
2	A	2001	ZLK	C28-C03-C04	-2.42	117.99	120.49
2	B	2001	ZLK	C24-C10-C11	-2.41	119.26	121.95
2	A	2001	ZLK	C26-C27-C28	2.40	122.03	119.25
2	B	2001	ZLK	C18-O17-C15	2.38	119.92	116.52
2	A	2001	ZLK	C11-C06-C07	2.38	108.50	106.34
2	B	2001	ZLK	C09-N08-C07	-2.37	123.20	125.70
2	A	2001	ZLK	C26-C25-C04	-2.37	118.29	121.39
2	A	2001	ZLK	C41-C40-C35	-2.34	121.95	124.17
2	B	2019	ZLK	C25-C26-C27	-2.28	118.36	120.80
2	B	2001	ZLK	C05-C04-C25	-2.28	116.34	120.06
2	B	2019	ZLK	C11-C06-C07	2.26	108.40	106.34
2	B	2019	ZLK	C13-N14-C15	-2.24	122.84	126.39
2	B	2001	ZLK	C10-N08-C07	2.24	110.17	108.54
2	B	2001	ZLK	C10-C11-C06	-2.22	105.35	107.39
3	B	2010	OLC	O20-C1-C2	2.22	121.00	114.00
2	A	2001	ZLK	O33-S32-C35	2.21	111.34	107.68
2	B	2001	ZLK	C36-C35-C40	-2.19	119.19	121.17
2	B	2019	ZLK	C27-C29-N31	2.19	118.69	116.08
2	A	2001	ZLK	O16-C15-N14	-2.17	121.51	126.12
2	B	2001	ZLK	O34-S32-C35	2.13	111.20	107.68
2	B	2001	ZLK	O02-C03-C28	-2.04	120.56	124.08

There are no chirality outliers.

All (221) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2019	ZLK	N14-C15-O17-C18
2	B	2019	ZLK	O16-C15-O17-C18

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Mol	Chain	Res	Type	Atoms
2	B	2019	ZLK	C19-C18-O17-C15
3	A	2007	OLC	C21-C22-C24-O25
3	B	2007	OLC	C10-C11-C12-C13
3	B	2009	OLC	C21-C22-C24-O25
3	A	2007	OLC	O19-C1-O20-C21
3	A	2007	OLC	C2-C1-O20-C21
5	A	2021	1PE	OH4-C13-C23-OH3
3	B	2009	OLC	C2-C1-O20-C21
3	B	2009	OLC	O20-C21-C22-C24
4	A	2014	OLA	C1-C2-C3-C4
3	B	2009	OLC	O19-C1-O20-C21
3	B	2009	OLC	O20-C21-C22-O23
4	A	2019	OLA	C1-C2-C3-C4
4	B	2015	OLA	C1-C2-C3-C4
3	B	2010	OLC	C1-C2-C3-C4
4	A	2013	OLA	C1-C2-C3-C4
4	A	2017	OLA	C1-C2-C3-C4
4	B	2017	OLA	C1-C2-C3-C4
4	B	2014	OLA	C1-C2-C3-C4
3	A	2007	OLC	C1-C2-C3-C4
4	B	2018	OLA	C1-C2-C3-C4
5	A	2021	1PE	OH2-C12-C22-OH3
4	A	2016	OLA	C1-C2-C3-C4
3	A	2003	OLC	C11-C12-C13-C14
4	A	2016	OLA	C12-C13-C14-C15
3	B	2009	OLC	O23-C22-C24-O25
3	A	2004	OLC	C5-C6-C7-C8
4	A	2011	OLA	C3-C4-C5-C6
4	A	2017	OLA	C4-C5-C6-C7
3	B	2009	OLC	C12-C13-C14-C15
4	A	2016	OLA	C3-C4-C5-C6
4	A	2019	OLA	C13-C14-C15-C16
3	A	2007	OLC	C4-C5-C6-C7
4	B	2013	OLA	C3-C4-C5-C6
4	B	2018	OLA	C14-C15-C16-C17
4	A	2012	OLA	C1-C2-C3-C4
3	B	2003	OLC	C4-C5-C6-C7
3	A	2003	OLC	C4-C5-C6-C7
3	A	2003	OLC	C3-C4-C5-C6
4	B	2013	OLA	C10-C11-C12-C13
3	A	2007	OLC	C3-C4-C5-C6
3	B	2009	OLC	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
4	A	2012	OLA	C2-C3-C4-C5
4	A	2013	OLA	C2-C3-C4-C5
4	A	2013	OLA	C4-C5-C6-C7
4	A	2016	OLA	C13-C14-C15-C16
4	A	2013	OLA	C12-C13-C14-C15
4	A	2019	OLA	C11-C12-C13-C14
4	B	2018	OLA	C4-C5-C6-C7
3	A	2003	OLC	C13-C14-C15-C16
3	A	2007	OLC	C5-C6-C7-C8
4	B	2017	OLA	C2-C3-C4-C5
4	A	2019	OLA	C14-C15-C16-C17
3	A	2002	OLC	C6-C7-C8-C9
3	B	2003	OLC	C6-C7-C8-C9
4	A	2013	OLA	C10-C11-C12-C13
4	A	2016	OLA	C6-C7-C8-C9
4	A	2011	OLA	C5-C6-C7-C8
4	B	2018	OLA	C3-C4-C5-C6
4	A	2011	OLA	C2-C3-C4-C5
3	B	2005	OLC	C6-C7-C8-C9
3	A	2007	OLC	C2-C3-C4-C5
4	B	2018	OLA	C13-C14-C15-C16
4	A	2020	OLA	C3-C4-C5-C6
2	B	2019	ZLK	O17-C15-N14-C13
4	B	2017	OLA	C3-C4-C5-C6
4	B	2017	OLA	C10-C11-C12-C13
3	A	2006	OLC	C13-C14-C15-C16
3	A	2009	OLC	C4-C5-C6-C7
3	B	2007	OLC	C6-C7-C8-C9
4	B	2016	OLA	C5-C6-C7-C8
4	A	2013	OLA	C13-C14-C15-C16
3	A	2002	OLC	C10-C11-C12-C13
3	B	2005	OLC	C10-C11-C12-C13
4	A	2013	OLA	C5-C6-C7-C8
4	A	2016	OLA	C4-C5-C6-C7
4	A	2019	OLA	C10-C11-C12-C13
4	B	2018	OLA	C6-C7-C8-C9
4	A	2017	OLA	C3-C4-C5-C6
4	B	2011	OLA	C3-C4-C5-C6
4	B	2016	OLA	C11-C12-C13-C14
3	B	2009	OLC	C5-C6-C7-C8
2	B	2019	ZLK	C29-N31-S32-O34
4	A	2019	OLA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	A	2007	OLC	C6-C7-C8-C9
3	A	2009	OLC	C2-C3-C4-C5
4	A	2010	OLA	C6-C7-C8-C9
4	A	2012	OLA	C3-C4-C5-C6
3	B	2005	OLC	C4-C5-C6-C7
4	B	2016	OLA	C1-C2-C3-C4
3	A	2007	OLC	O23-C22-C24-O25
4	B	2013	OLA	C11-C12-C13-C14
4	B	2012	OLA	C5-C6-C7-C8
3	B	2007	OLC	C4-C5-C6-C7
4	B	2016	OLA	C15-C16-C17-C18
4	B	2017	OLA	C13-C14-C15-C16
4	B	2017	OLA	C12-C13-C14-C15
4	B	2011	OLA	C2-C3-C4-C5
4	B	2013	OLA	C1-C2-C3-C4
3	B	2009	OLC	C13-C14-C15-C16
4	B	2015	OLA	C6-C7-C8-C9
3	A	2003	OLC	C14-C15-C16-C17
3	B	2006	OLC	C11-C12-C13-C14
3	B	2010	OLC	C2-C3-C4-C5
3	B	2002	OLC	C6-C7-C8-C9
4	A	2020	OLA	C9-C10-C11-C12
3	A	2006	OLC	C15-C16-C17-C18
4	A	2013	OLA	C14-C15-C16-C17
4	B	2012	OLA	C4-C5-C6-C7
4	A	2013	OLA	C6-C7-C8-C9
3	A	2008	OLC	C6-C7-C8-C9
3	B	2004	OLC	C10-C11-C12-C13
3	B	2006	OLC	C5-C6-C7-C8
3	A	2006	OLC	C14-C15-C16-C17
4	B	2018	OLA	C15-C16-C17-C18
5	A	2021	1PE	C23-C13-OH4-C24
3	A	2003	OLC	C5-C6-C7-C8
2	B	2019	ZLK	C40-C35-S32-O34
4	B	2013	OLA	C2-C3-C4-C5
3	A	2003	OLC	C2-C3-C4-C5
4	A	2019	OLA	C5-C6-C7-C8
3	A	2009	OLC	C5-C6-C7-C8
4	A	2017	OLA	C2-C3-C4-C5
2	B	2001	ZLK	C40-C35-S32-O33
4	A	2016	OLA	C11-C12-C13-C14
3	B	2007	OLC	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	A	2005	OLC	C6-C7-C8-C9
3	A	2003	OLC	C12-C13-C14-C15
3	A	2003	OLC	C9-C10-C11-C12
3	B	2003	OLC	C3-C4-C5-C6
3	B	2004	OLC	C5-C6-C7-C8
3	B	2008	OLC	C5-C6-C7-C8
4	A	2018	OLA	C7-C8-C9-C10
4	A	2017	OLA	C5-C6-C7-C8
3	A	2002	OLC	C7-C8-C9-C10
4	A	2019	OLA	C7-C8-C9-C10
4	B	2012	OLA	C1-C2-C3-C4
4	B	2013	OLA	C6-C7-C8-C9
4	A	2016	OLA	C14-C15-C16-C17
3	B	2005	OLC	C7-C8-C9-C10
4	B	2015	OLA	C2-C3-C4-C5
4	A	2015	OLA	O2-C1-C2-C3
4	B	2018	OLA	C12-C13-C14-C15
4	A	2014	OLA	O1-C1-C2-C3
4	A	2014	OLA	O2-C1-C2-C3
4	A	2017	OLA	O1-C1-C2-C3
3	B	2010	OLC	O19-C1-C2-C3
4	A	2015	OLA	O1-C1-C2-C3
3	B	2006	OLC	C7-C8-C9-C10
4	A	2016	OLA	O2-C1-C2-C3
3	B	2010	OLC	O20-C1-C2-C3
4	B	2014	OLA	O2-C1-C2-C3
4	B	2011	OLA	O2-C1-C2-C3
4	B	2014	OLA	O1-C1-C2-C3
3	A	2002	OLC	C9-C10-C11-C12
4	A	2013	OLA	O2-C1-C2-C3
4	A	2019	OLA	O2-C1-C2-C3
4	B	2012	OLA	O2-C1-C2-C3
4	A	2017	OLA	O2-C1-C2-C3
2	B	2019	ZLK	O16-C15-N14-C13
4	A	2013	OLA	O1-C1-C2-C3
4	B	2012	OLA	O1-C1-C2-C3
4	B	2018	OLA	O1-C1-C2-C3
4	A	2011	OLA	C4-C5-C6-C7
4	B	2014	OLA	C2-C3-C4-C5
4	B	2015	OLA	O1-C1-C2-C3
4	B	2018	OLA	C10-C11-C12-C13
4	A	2019	OLA	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	B	2011	OLA	O1-C1-C2-C3
4	B	2017	OLA	O2-C1-C2-C3
4	B	2017	OLA	O1-C1-C2-C3
4	A	2012	OLA	O1-C1-C2-C3
4	A	2016	OLA	O1-C1-C2-C3
4	B	2018	OLA	O2-C1-C2-C3
4	A	2012	OLA	O2-C1-C2-C3
4	B	2014	OLA	C3-C4-C5-C6
4	B	2015	OLA	O2-C1-C2-C3
3	B	2009	OLC	C6-C7-C8-C9
2	B	2019	ZLK	C03-C04-C05-C06
4	A	2020	OLA	C7-C8-C9-C10
4	A	2016	OLA	C15-C16-C17-C18
4	B	2017	OLA	C6-C7-C8-C9
3	A	2009	OLC	C3-C4-C5-C6
4	B	2013	OLA	O2-C1-C2-C3
3	A	2008	OLC	C7-C8-C9-C10
3	B	2004	OLC	C7-C8-C9-C10
3	B	2004	OLC	C4-C5-C6-C7
4	A	2010	OLA	C4-C5-C6-C7
3	A	2008	OLC	C9-C10-C11-C12
3	B	2009	OLC	C9-C10-C11-C12
4	A	2019	OLA	C9-C10-C11-C12
4	B	2016	OLA	O2-C1-C2-C3
4	B	2013	OLA	O1-C1-C2-C3
2	A	2001	ZLK	C22-C18-O17-C15
2	A	2001	ZLK	C40-C35-S32-O33
4	B	2016	OLA	O1-C1-C2-C3
3	B	2004	OLC	C9-C10-C11-C12
4	B	2017	OLA	C9-C10-C11-C12
3	B	2008	OLC	C6-C7-C8-C9
4	A	2010	OLA	O1-C1-C2-C3
4	A	2010	OLA	O2-C1-C2-C3
4	B	2016	OLA	C9-C10-C11-C12
4	B	2018	OLA	C7-C8-C9-C10
3	A	2006	OLC	C11-C12-C13-C14
4	B	2013	OLA	C9-C10-C11-C12
4	B	2013	OLA	C7-C8-C9-C10
4	A	2010	OLA	C5-C6-C7-C8
4	B	2012	OLA	C3-C4-C5-C6
4	A	2019	OLA	C15-C16-C17-C18
4	A	2011	OLA	O2-C1-C2-C3

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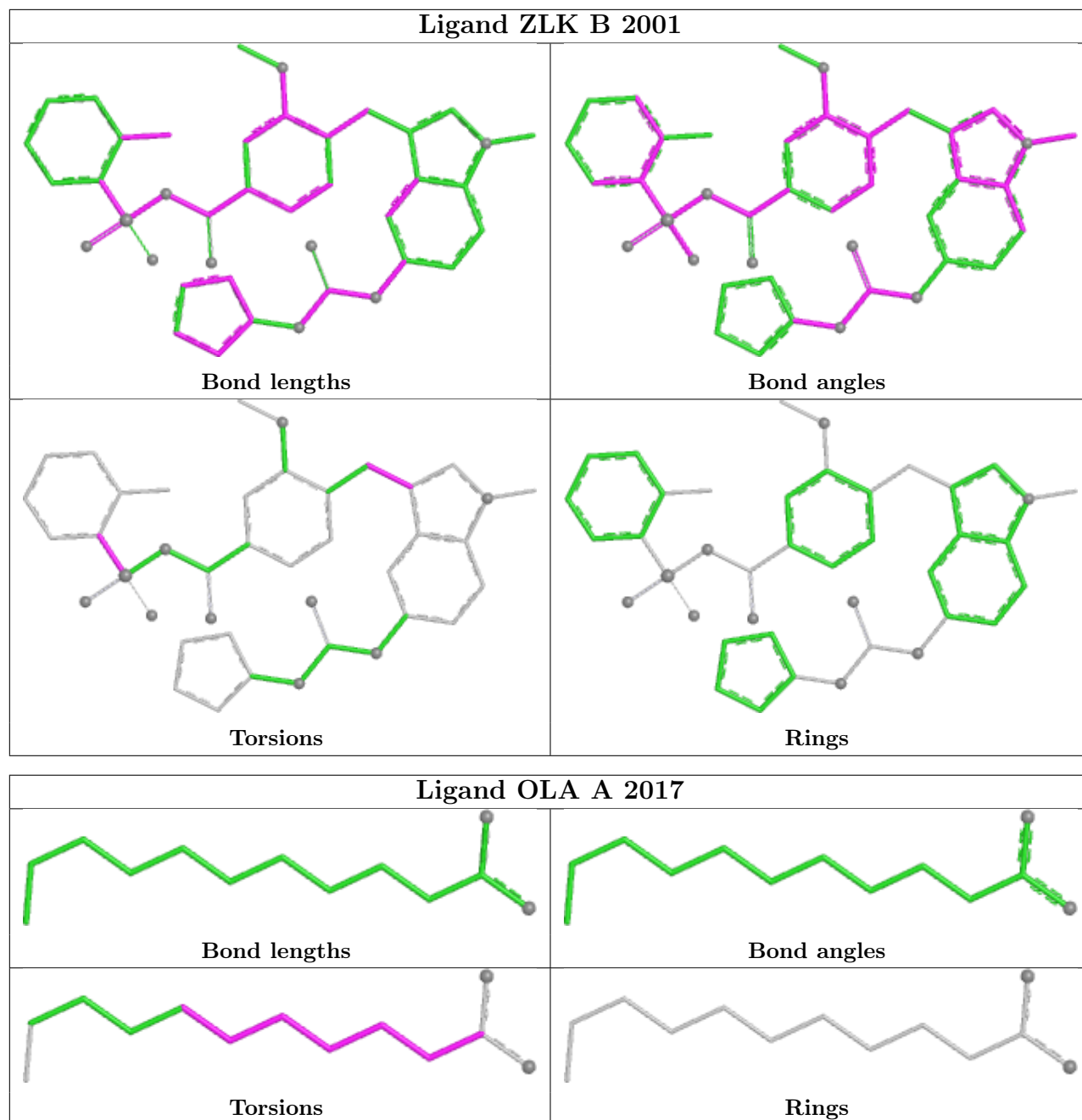
Mol	Chain	Res	Type	Atoms
5	A	2021	1PE	OH5-C14-C24-OH4
3	A	2006	OLC	C7-C8-C9-C10
4	A	2018	OLA	C9-C10-C11-C12
4	A	2011	OLA	O1-C1-C2-C3
2	B	2001	ZLK	C04-C05-C06-C07
3	B	2009	OLC	O20-C1-C2-C3
3	A	2004	OLC	C11-C12-C13-C14
3	A	2007	OLC	O20-C1-C2-C3
3	A	2005	OLC	C9-C10-C11-C12

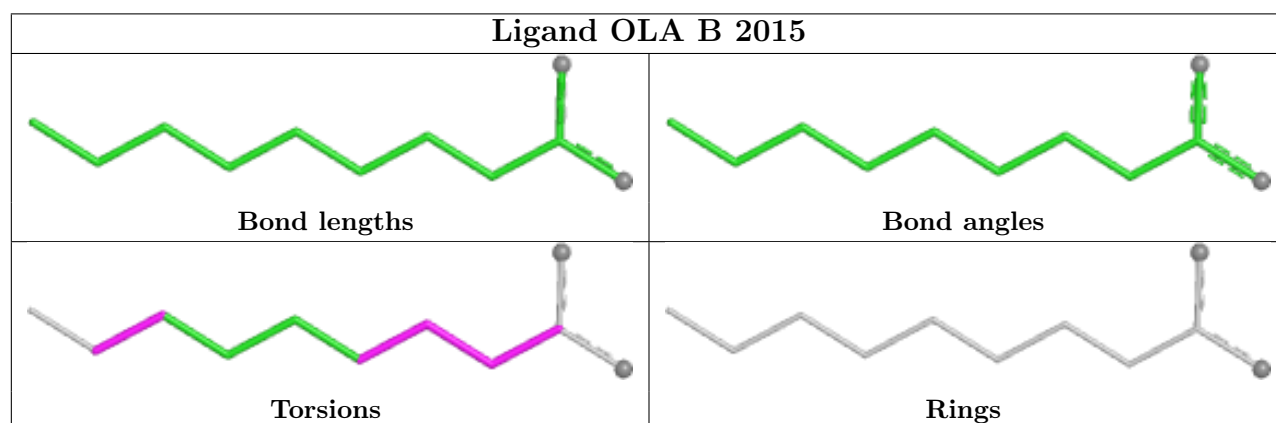
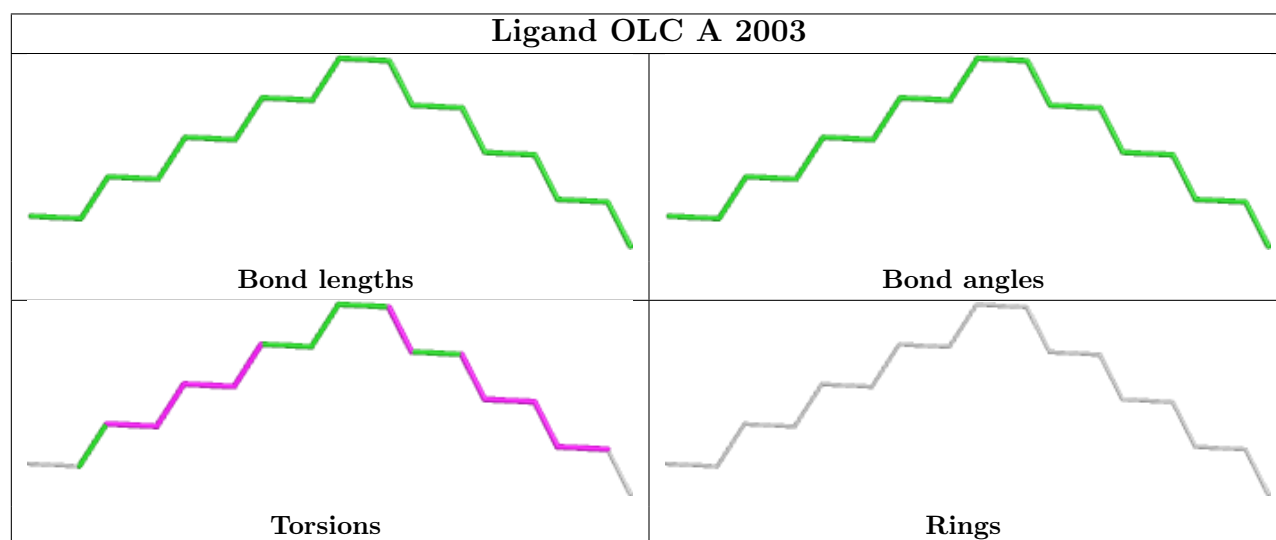
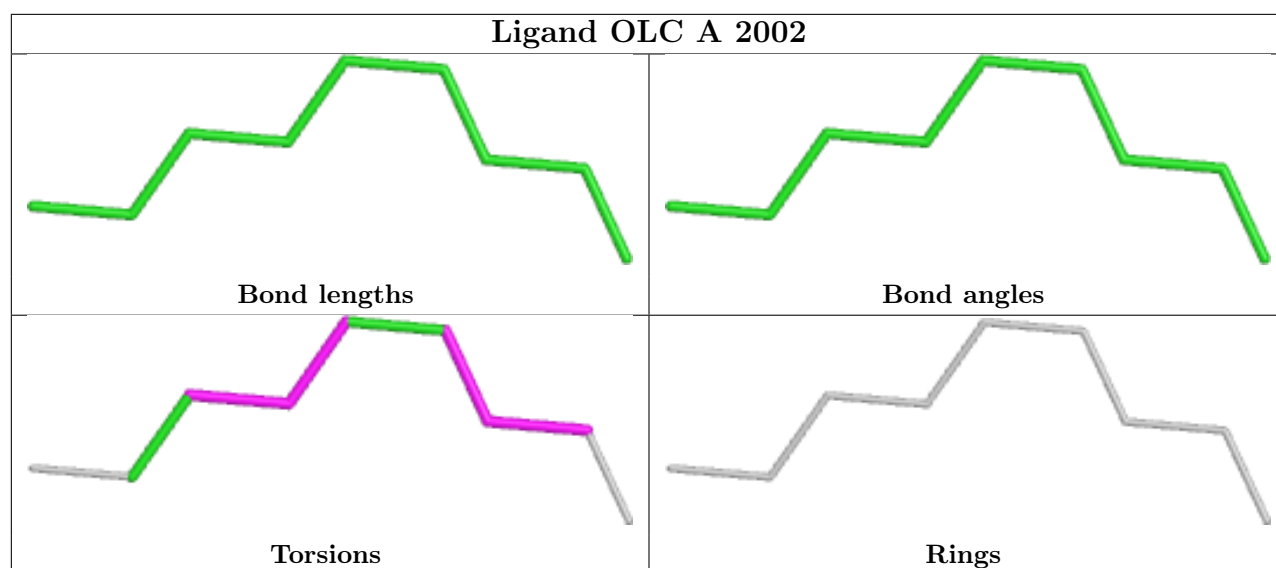
There are no ring outliers.

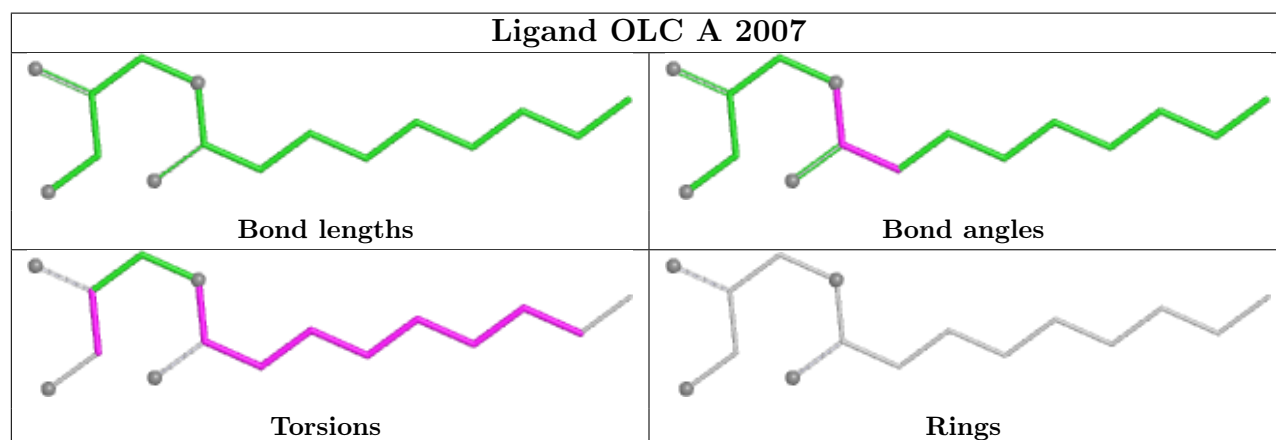
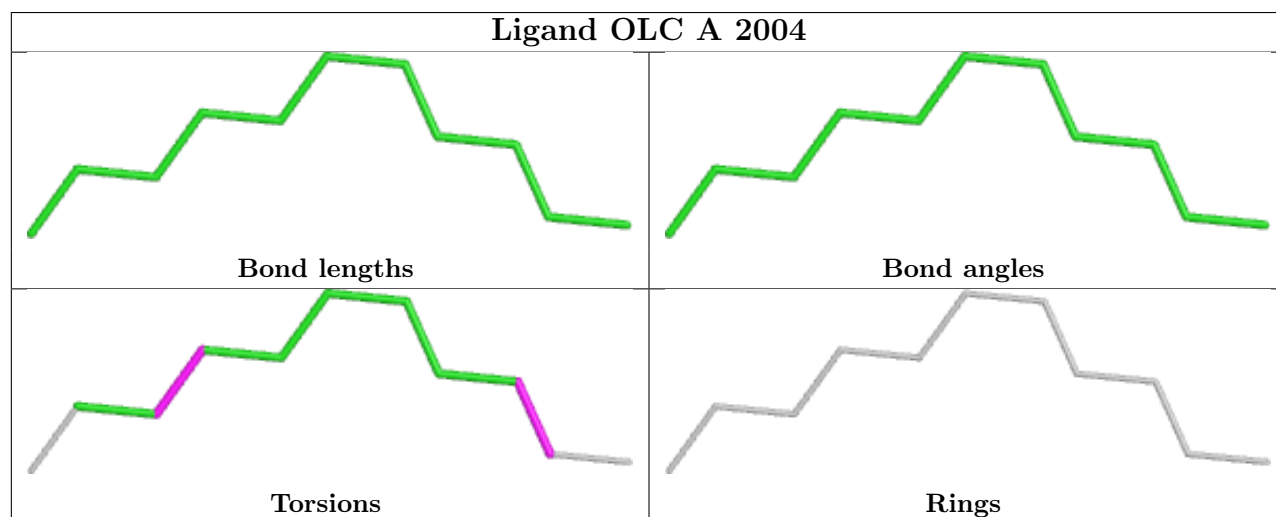
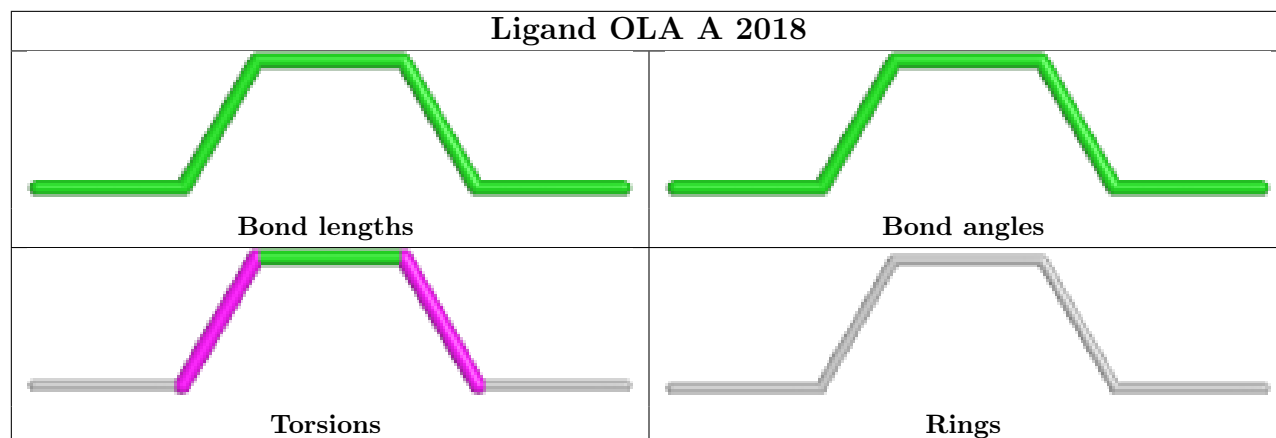
11 monomers are involved in 9 short contacts:

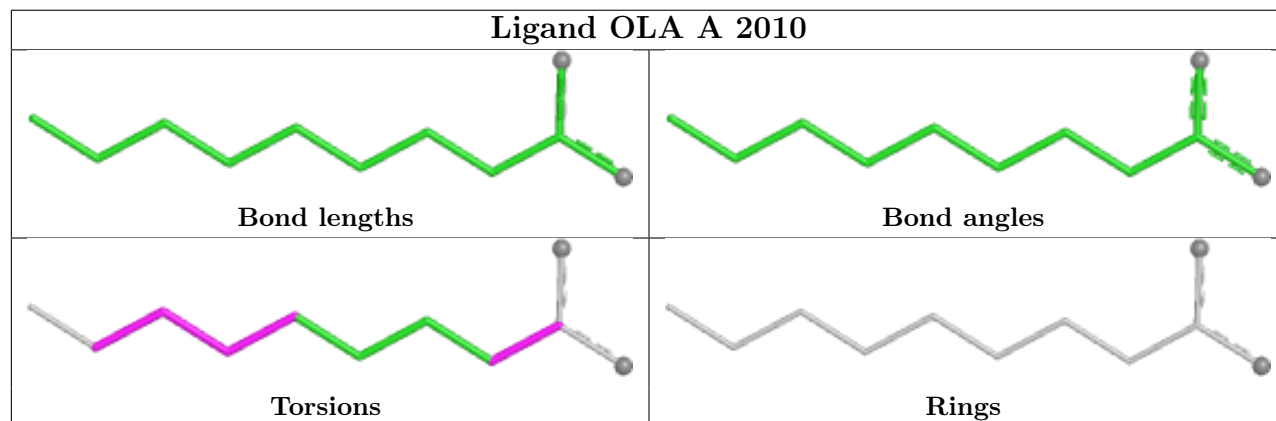
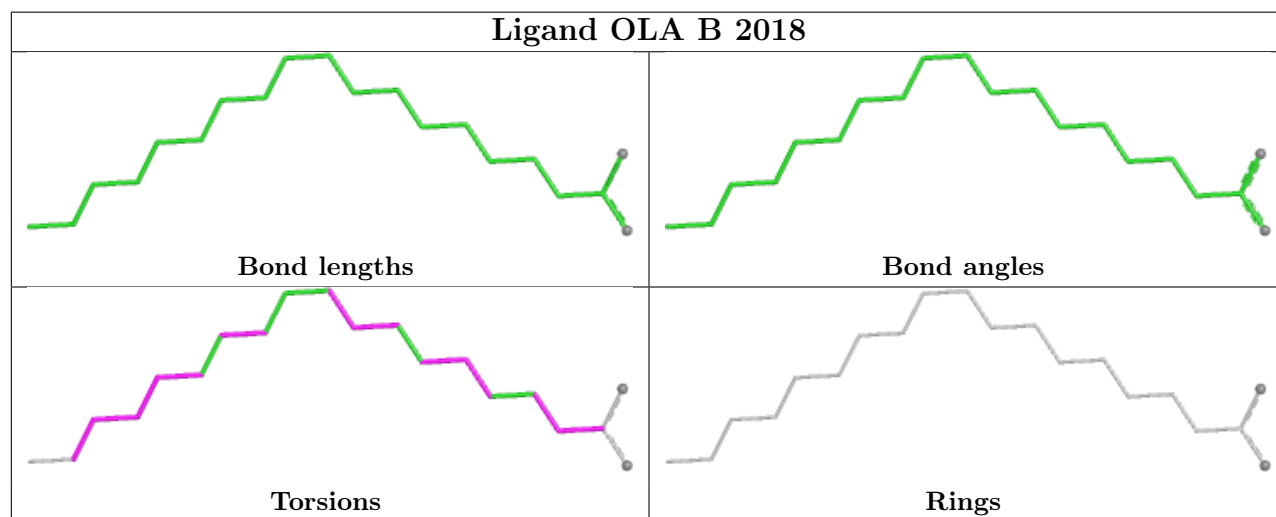
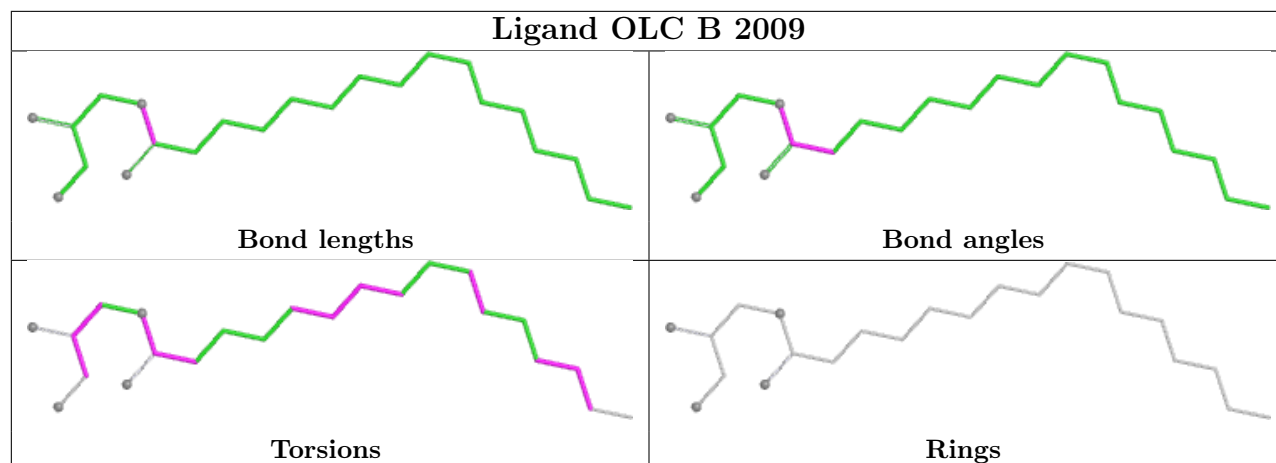
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2010	OLC	1	0
4	A	2012	OLA	1	0
4	B	2013	OLA	1	0
4	A	2014	OLA	2	0
4	B	2016	OLA	1	0
4	A	2019	OLA	2	0
4	B	2011	OLA	1	0
4	A	2013	OLA	1	0
4	B	2014	OLA	1	0
3	B	2004	OLC	1	0
3	B	2006	OLC	1	0

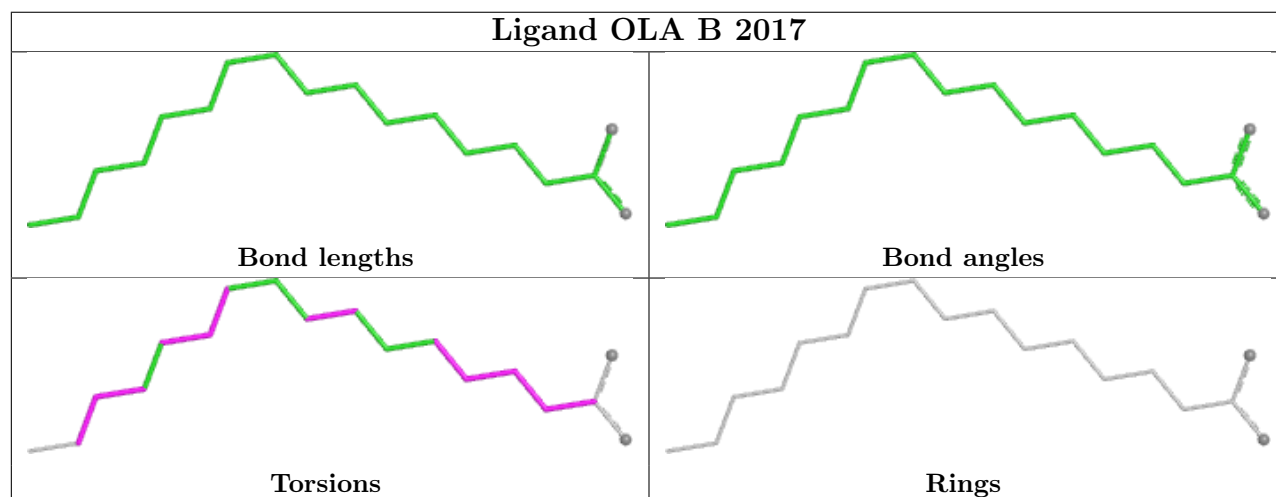
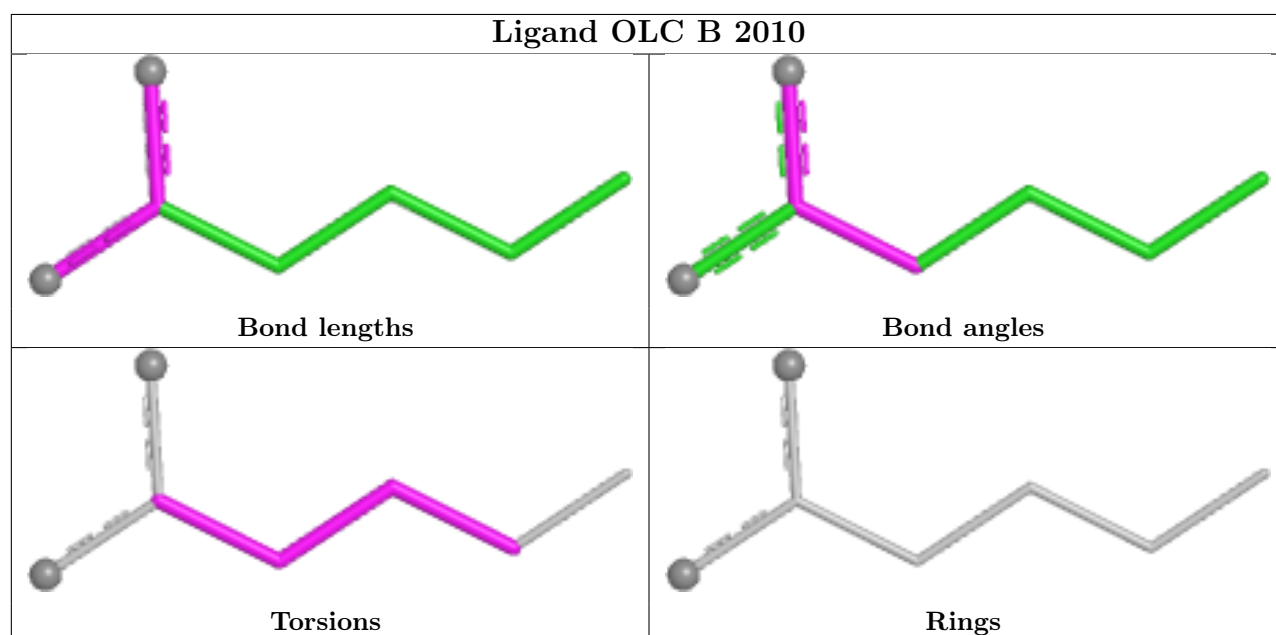
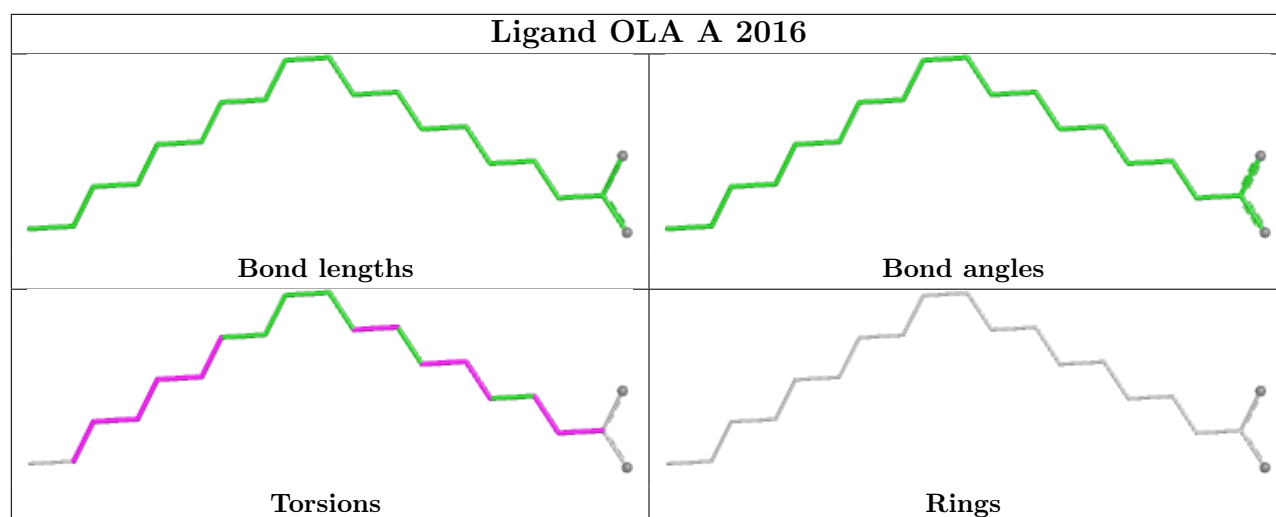
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

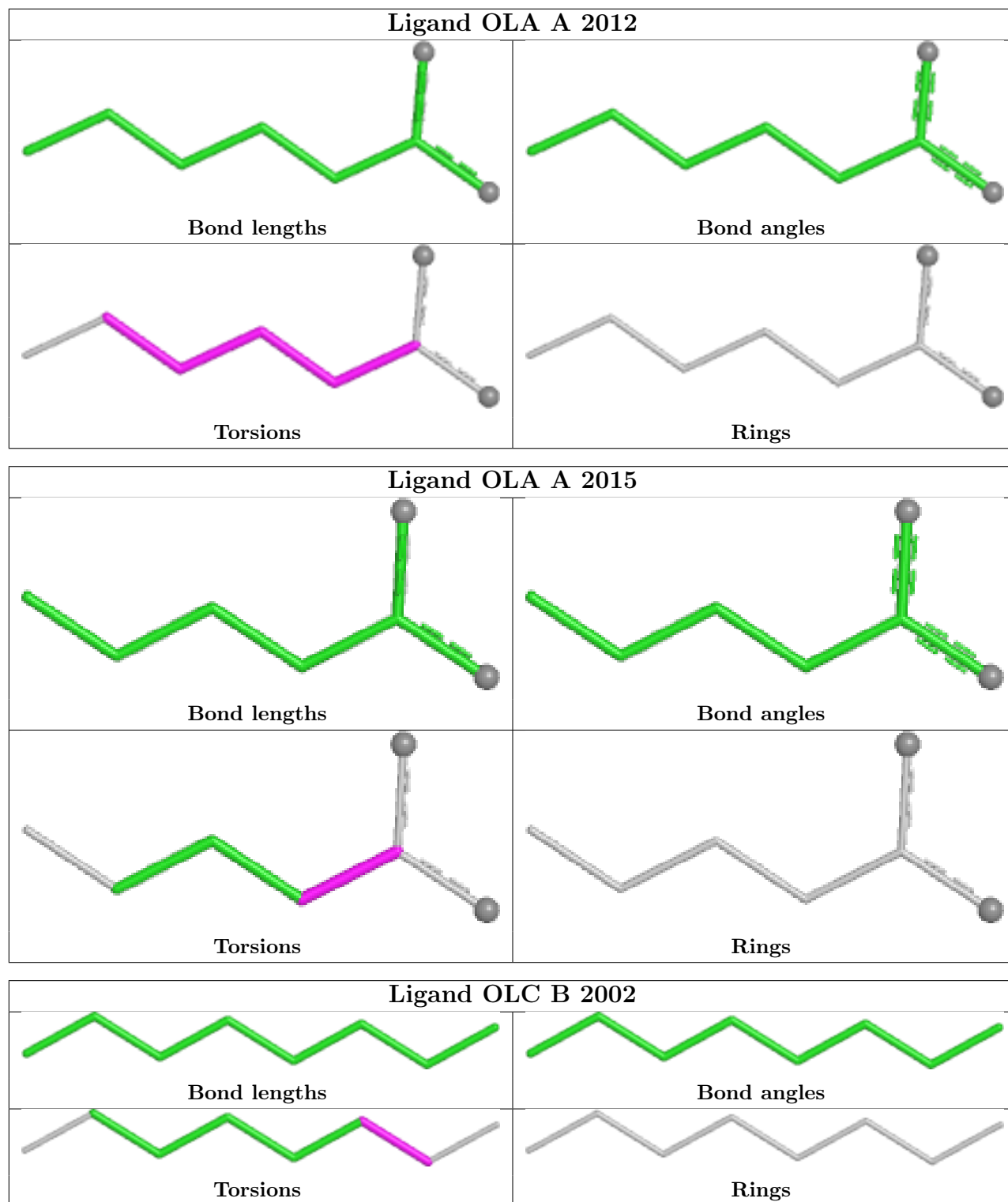


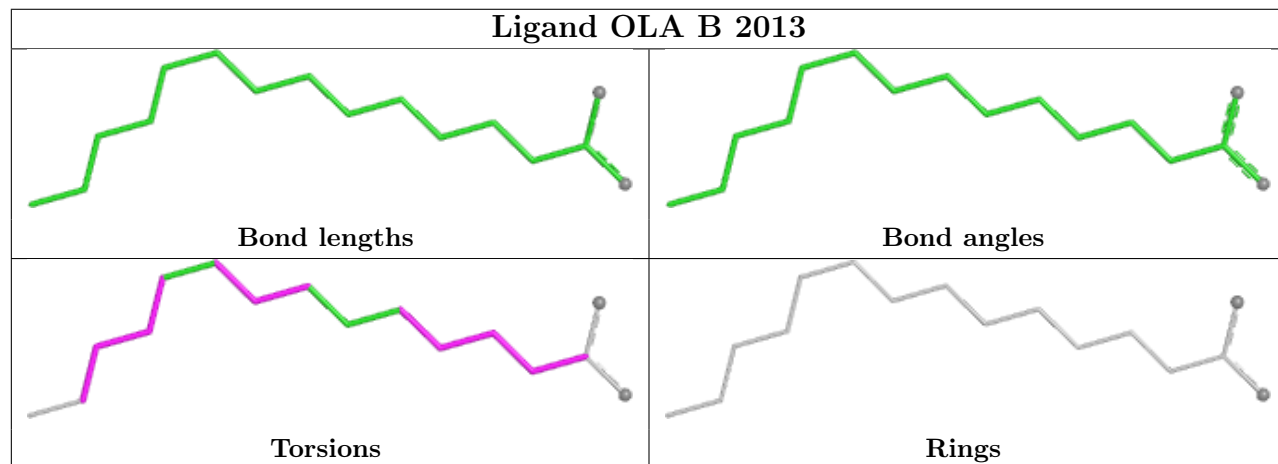
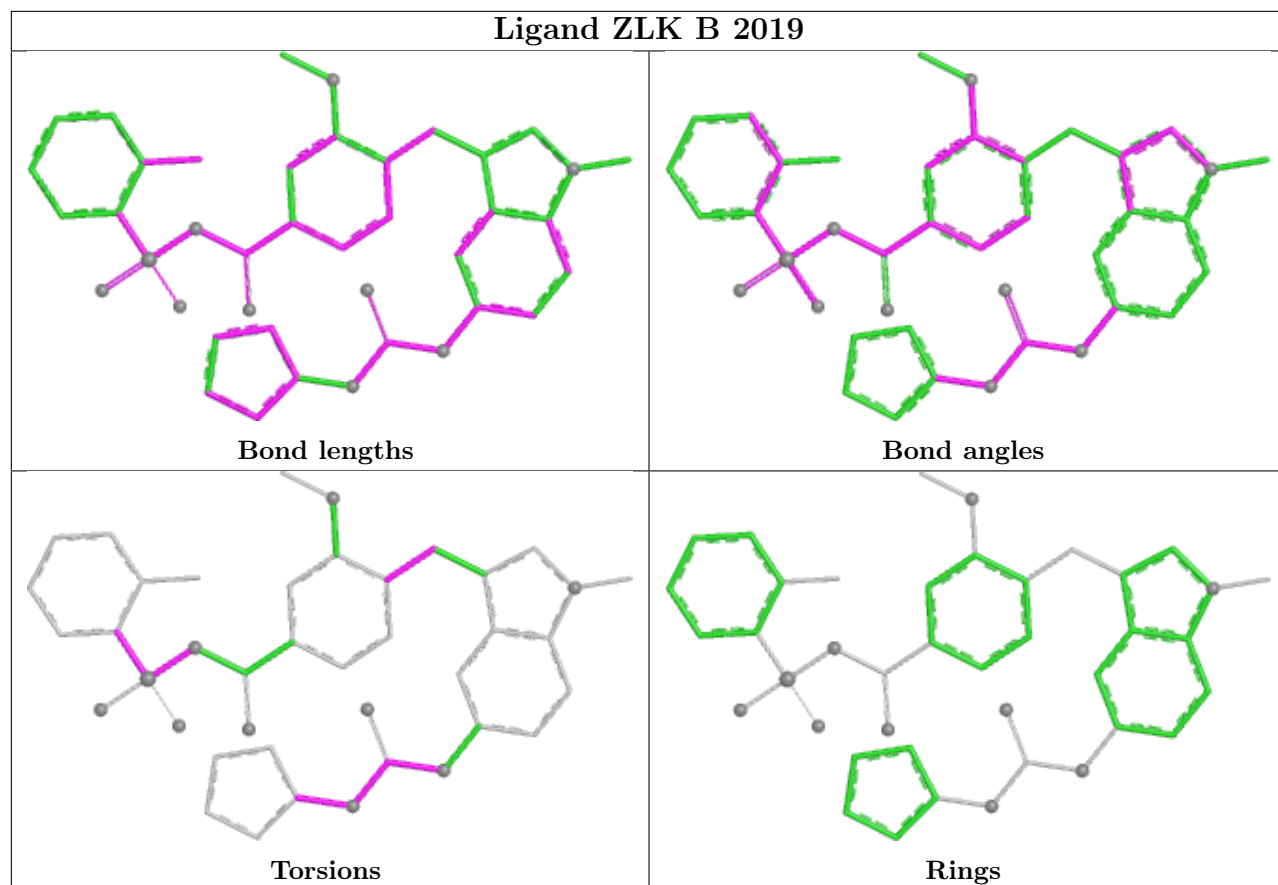


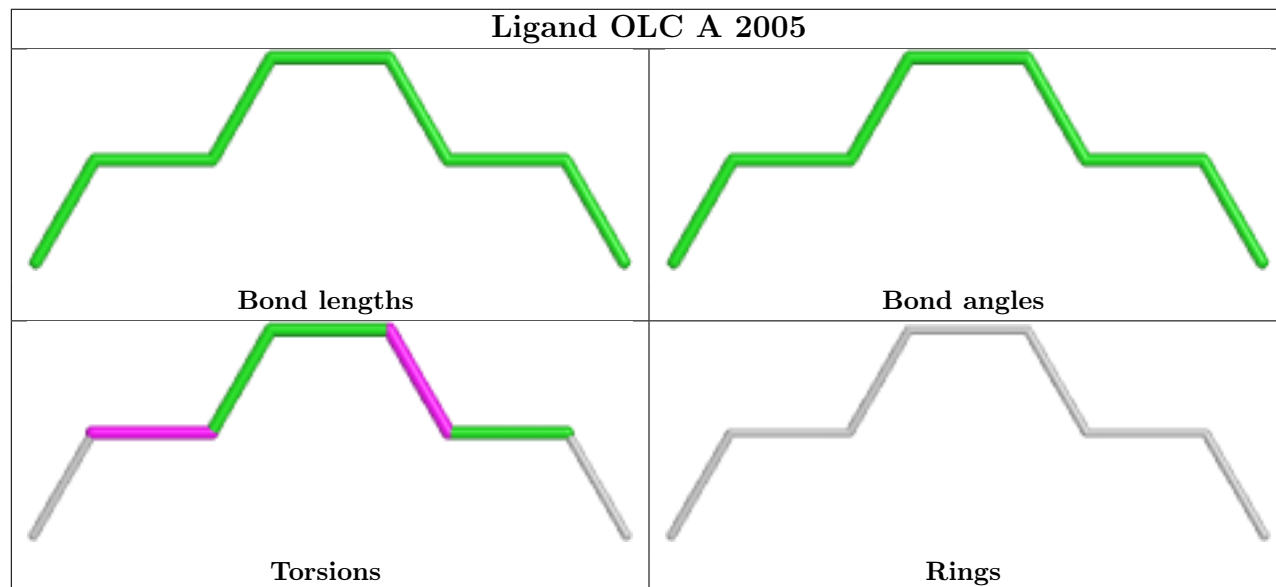
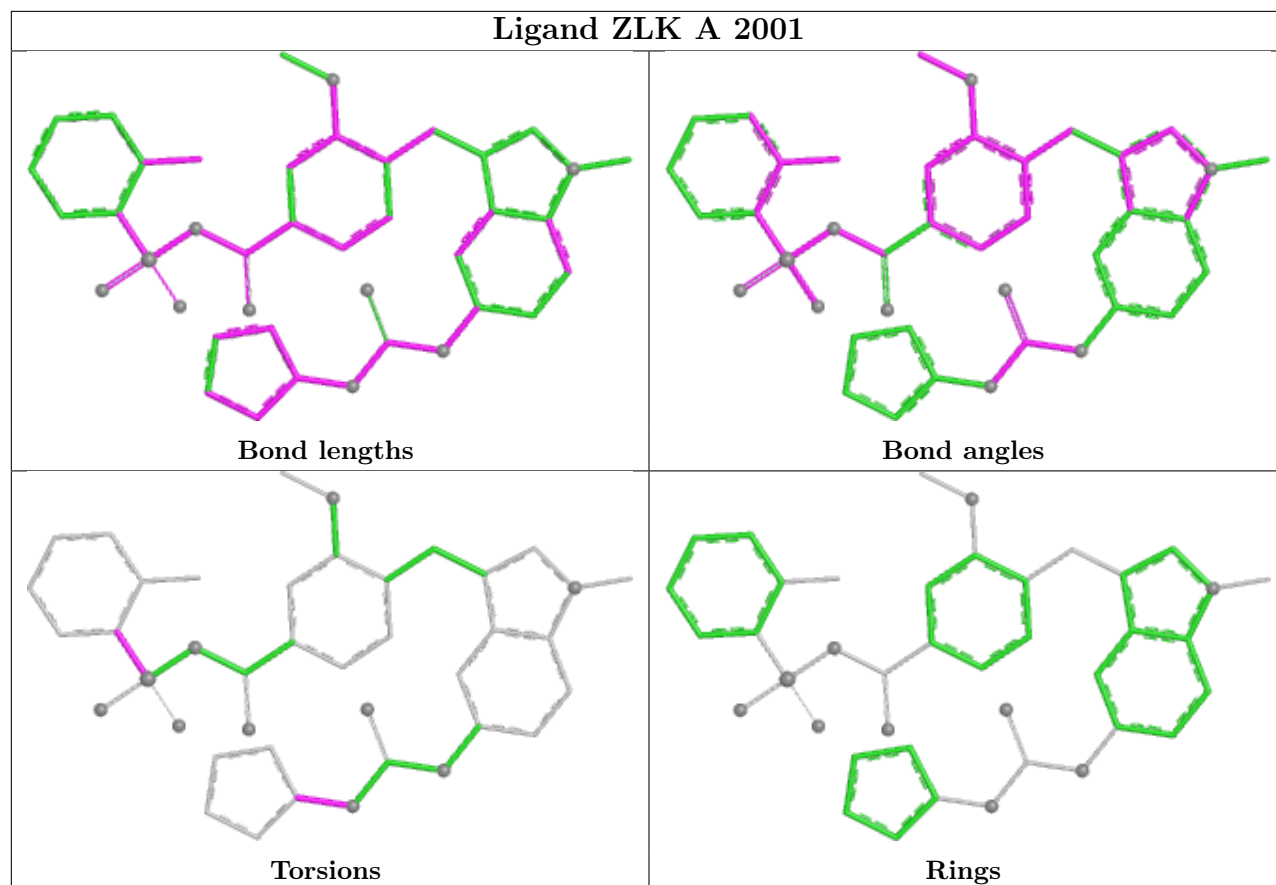


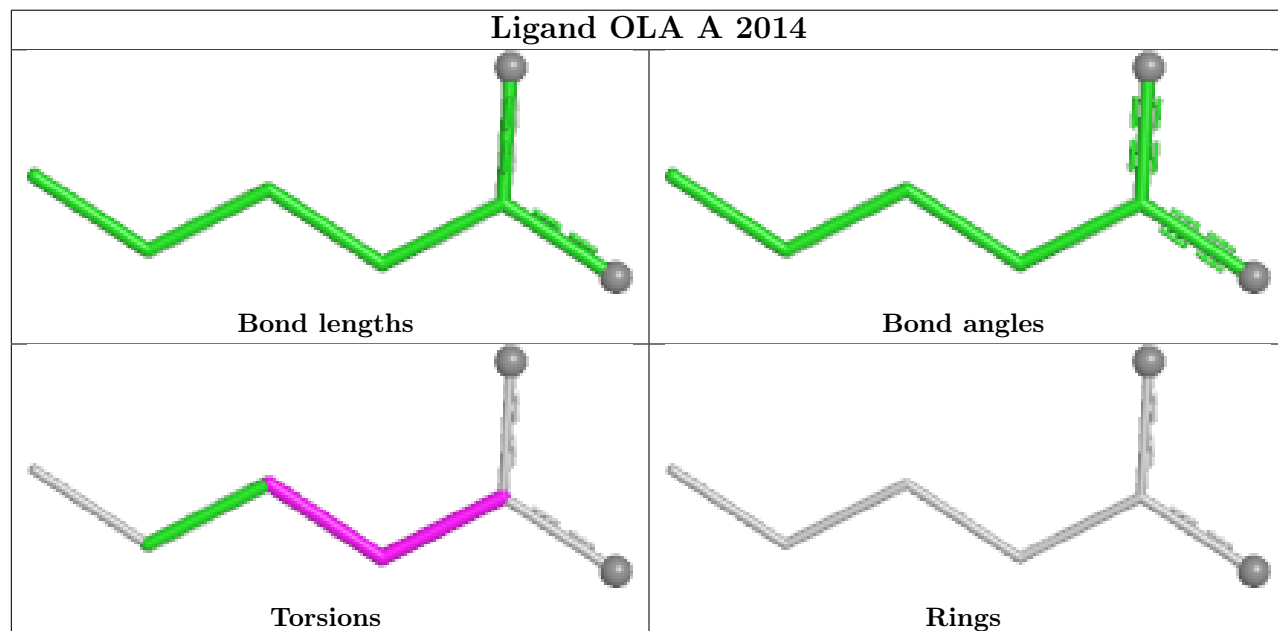
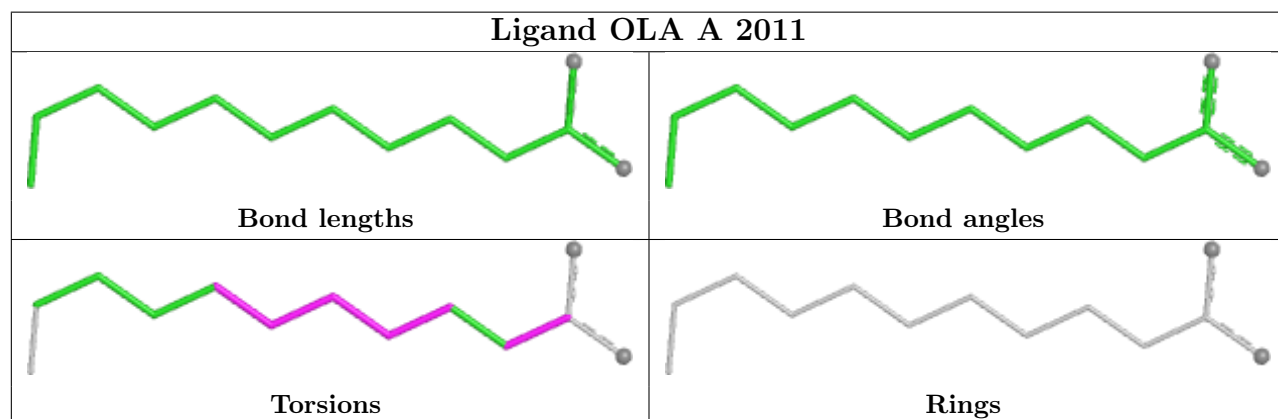
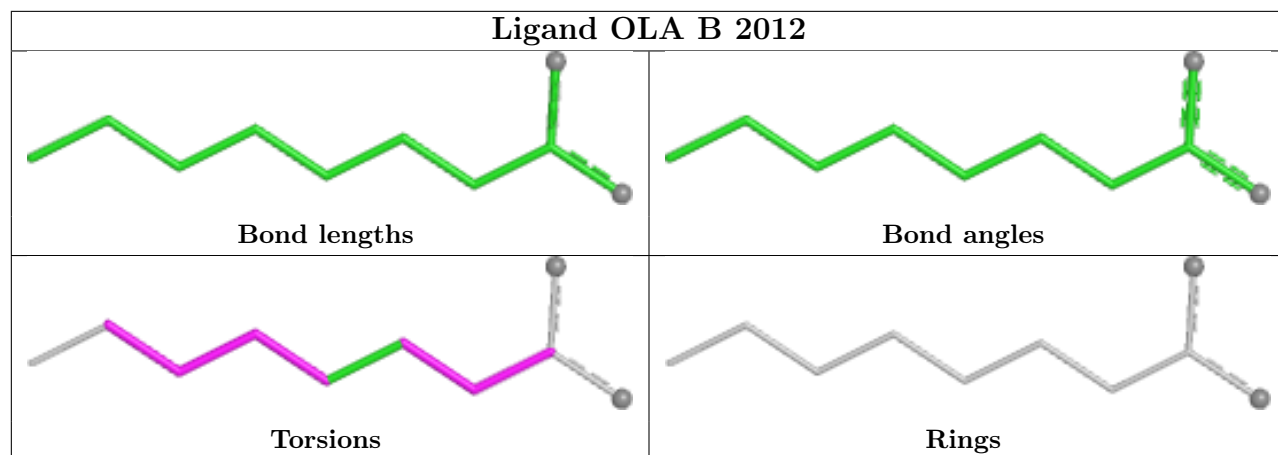


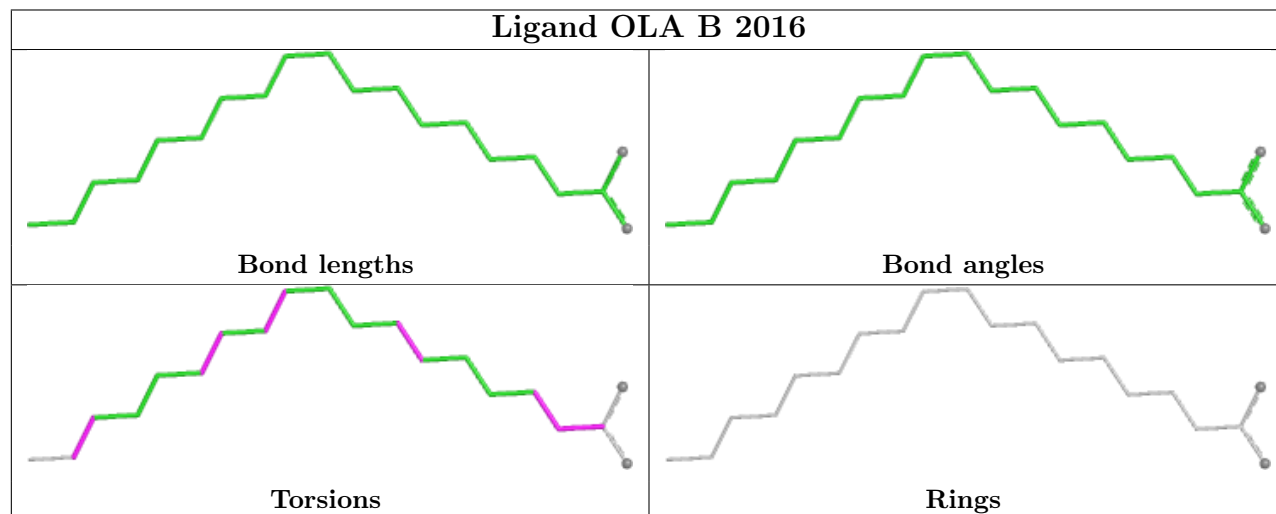
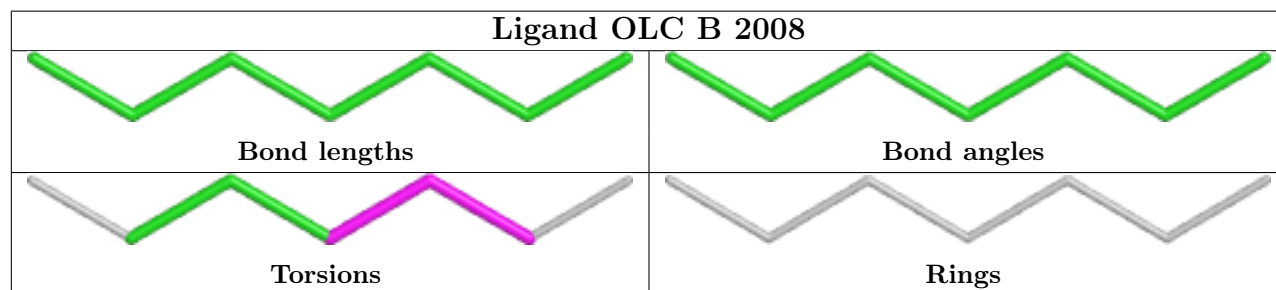
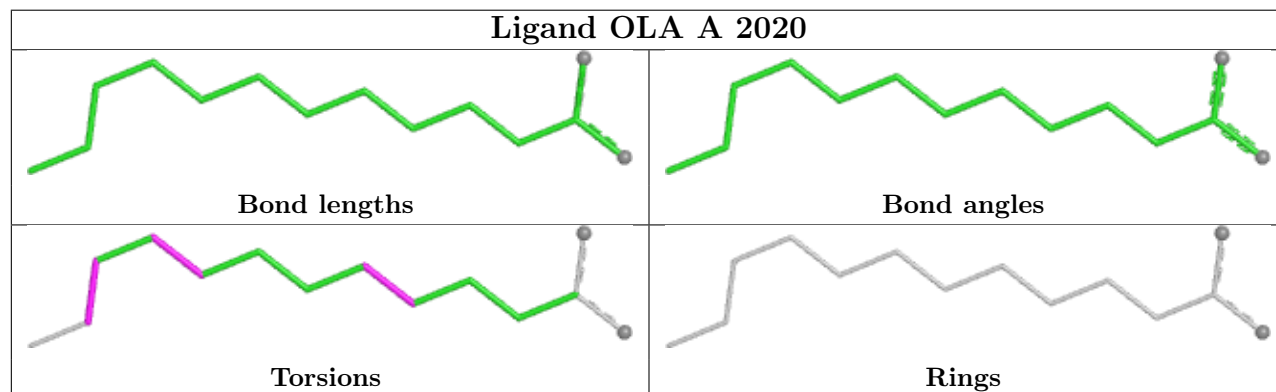
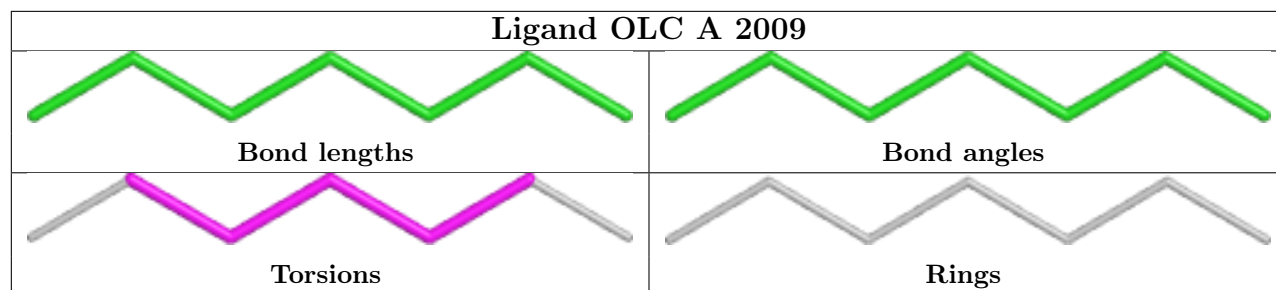


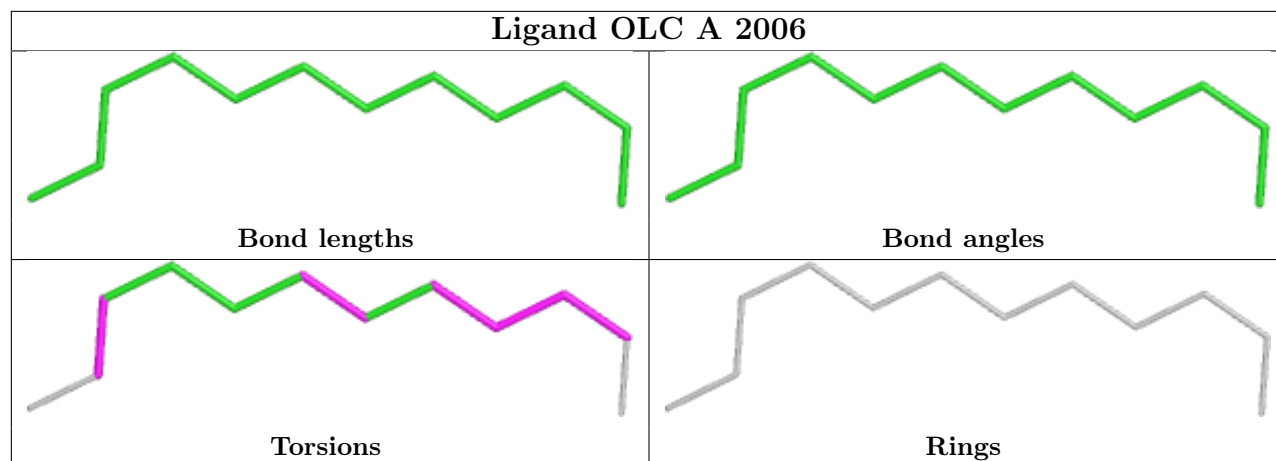
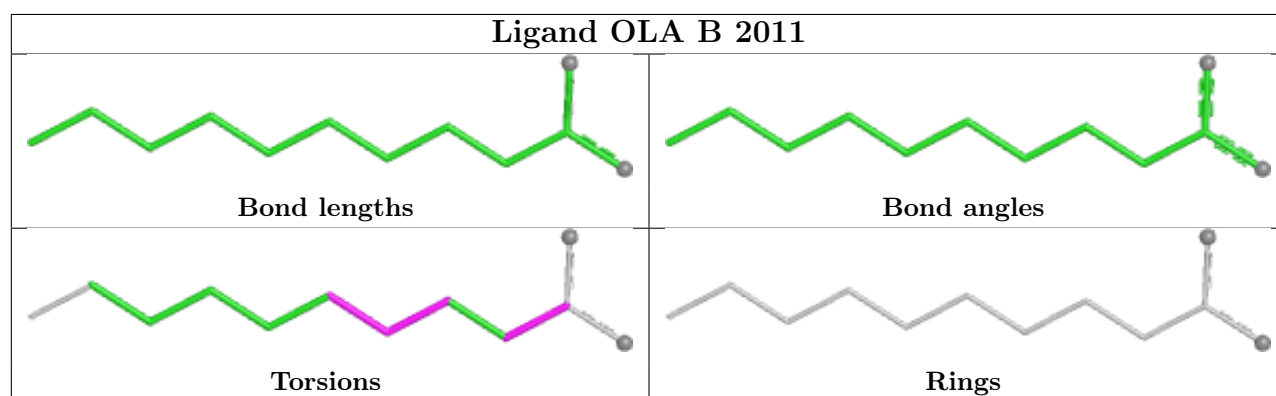
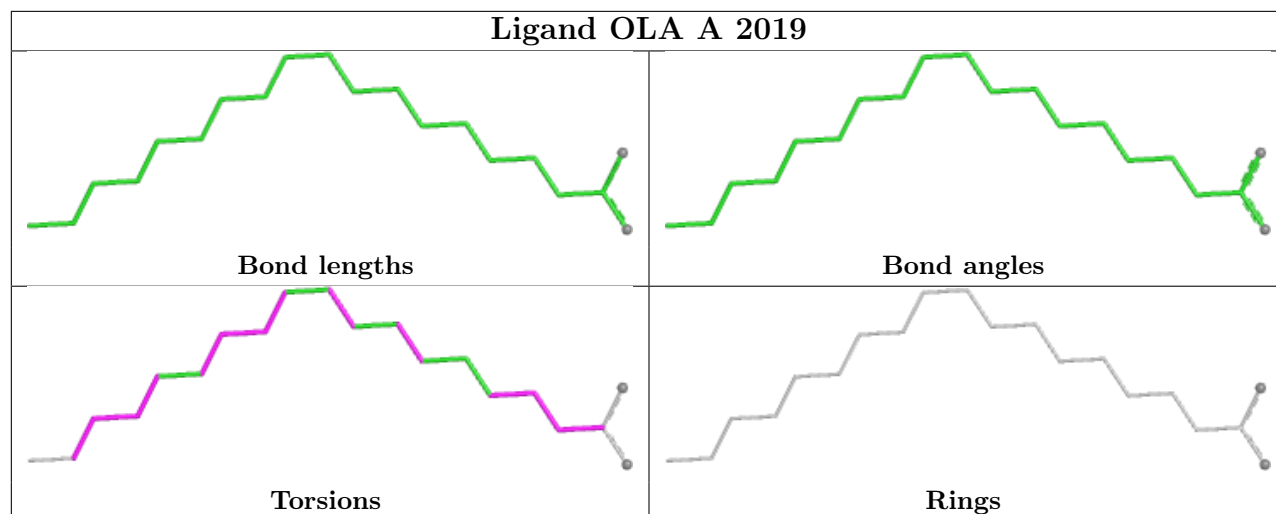


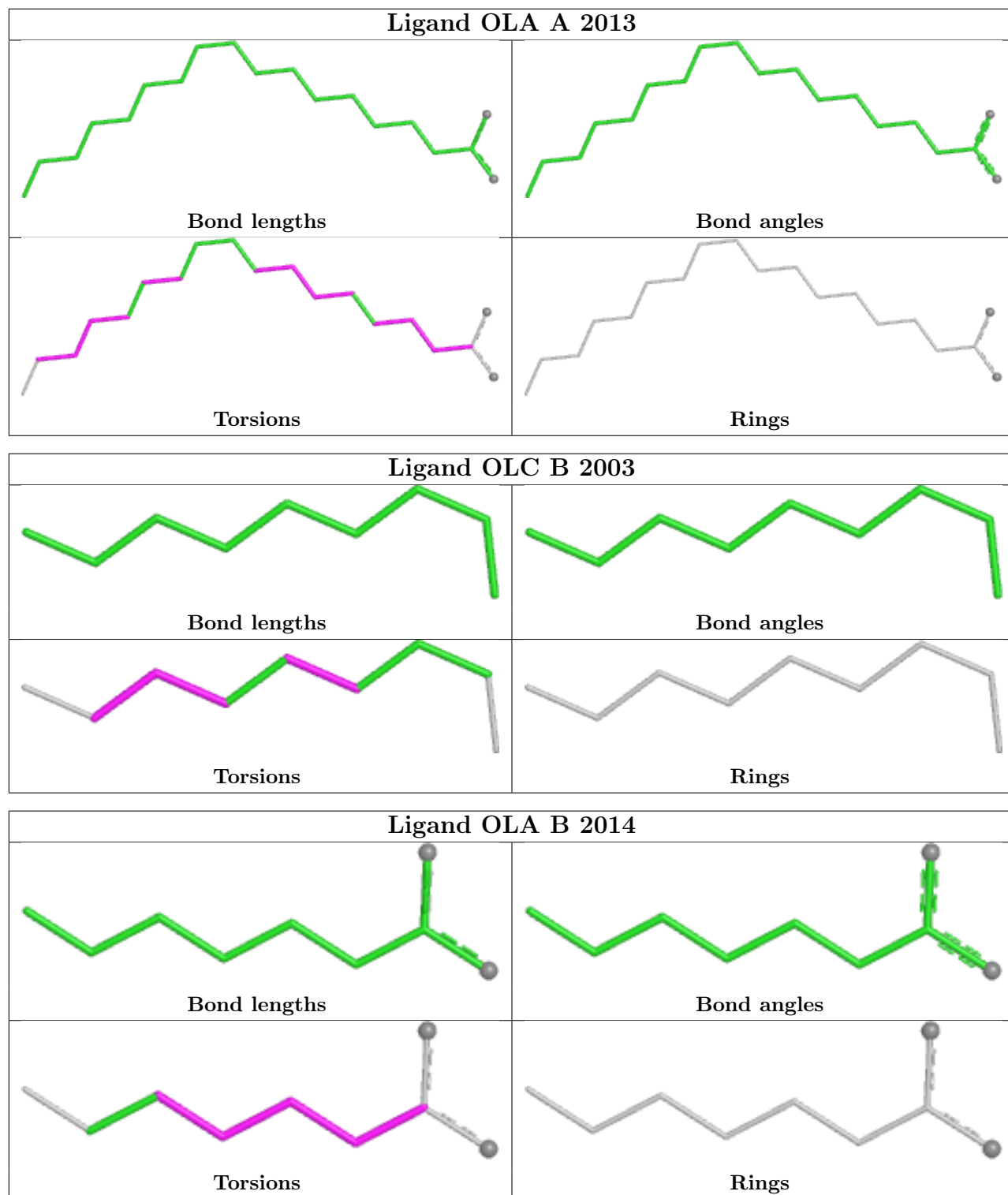


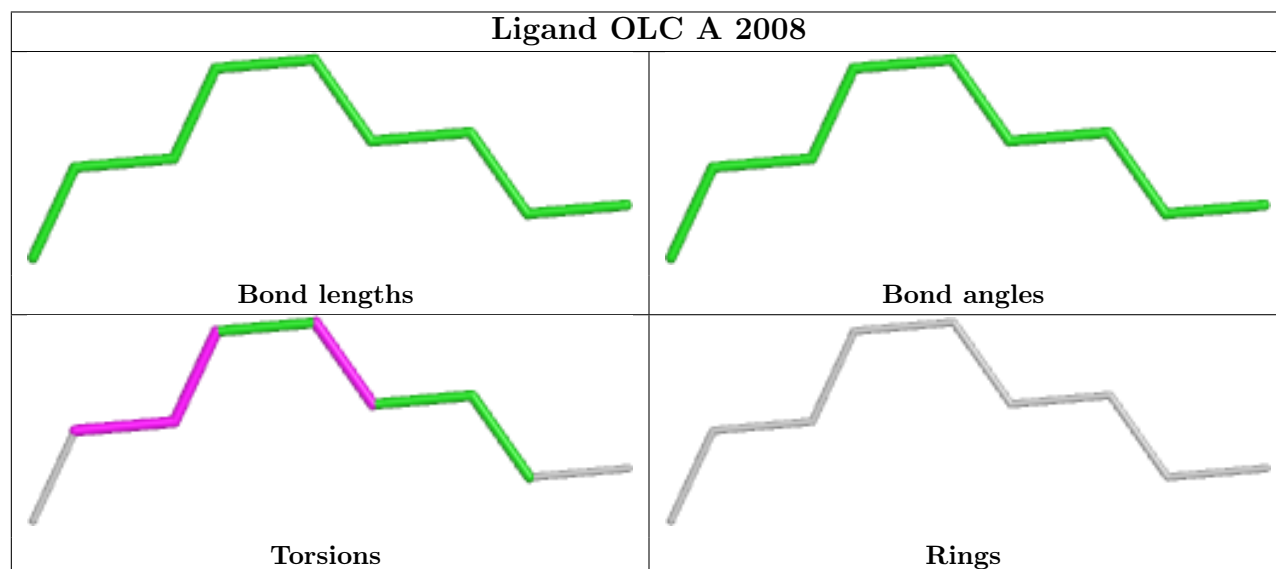
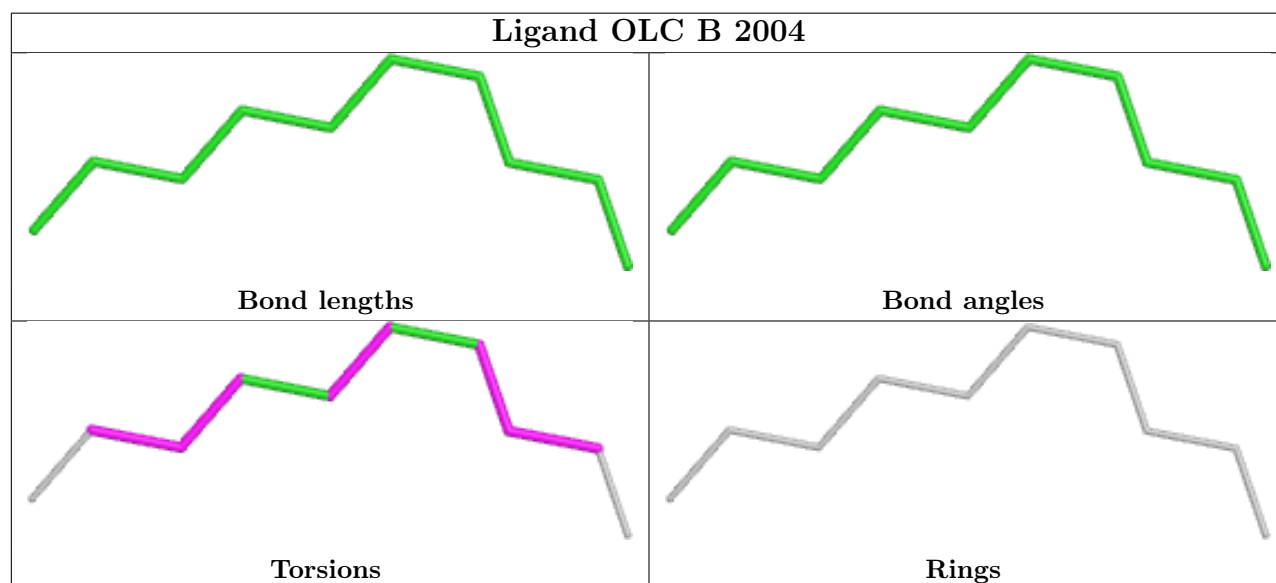
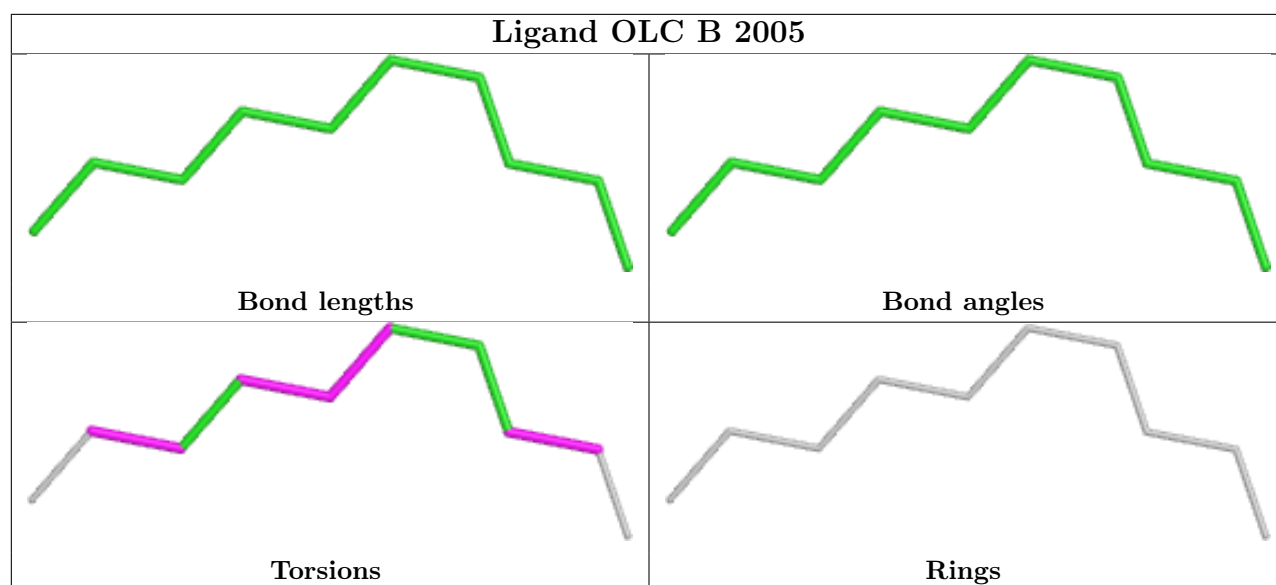


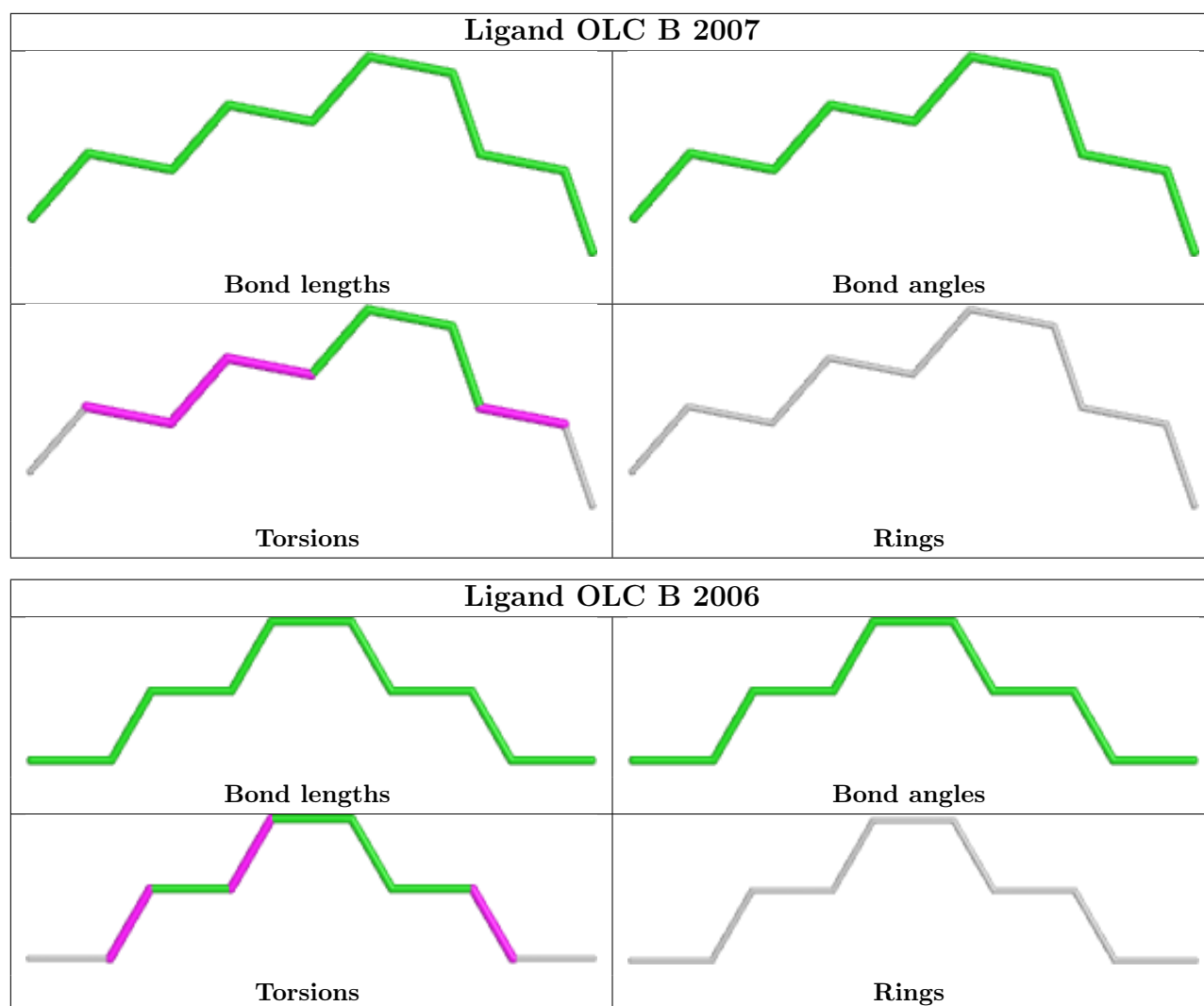












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	369/423 (87%)	0.14	4 (1%) 78 76	47, 81, 157, 171	1 (0%)
1	B	385/423 (91%)	0.32	9 (2%) 61 57	39, 93, 154, 179	2 (0%)
All	All	754/846 (89%)	0.23	13 (1%) 69 66	39, 87, 155, 179	3 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1007	TRP	3.6
1	B	1087	ALA	3.1
1	A	1101	TYR	3.1
1	B	1018	GLU	2.6
1	B	1068	LEU	2.6
1	B	1040	ALA	2.5
1	B	1003	LEU	2.4
1	A	177	PRO	2.3
1	B	1029	ALA	2.3
1	B	1064	GLY	2.3
1	B	1065	PHE	2.3
1	A	1061	PHE	2.2
1	A	1094	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

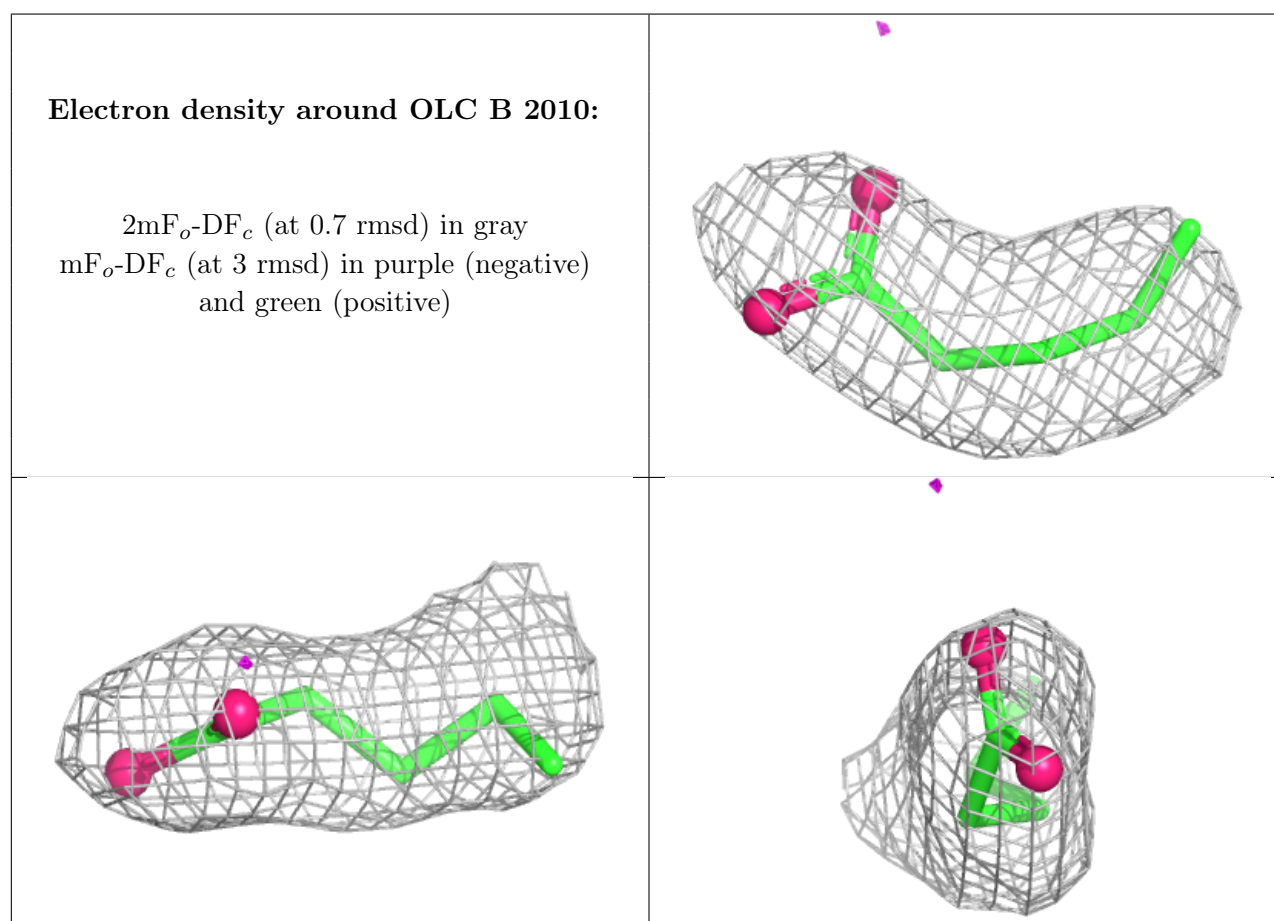
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OLC	B	2010	7/25	0.69	0.15	102,106,112,114	0
3	OLC	B	2002	8/25	0.75	0.12	79,80,82,82	0
4	OLA	A	2010	11/20	0.76	0.13	93,96,109,110	0
4	OLA	B	2018	20/20	0.78	0.16	120,122,131,131	0
4	OLA	B	2015	11/20	0.79	0.10	95,101,110,112	0
3	OLC	A	2003	17/25	0.79	0.15	73,96,100,100	0
4	OLA	A	2017	13/20	0.80	0.11	99,106,114,114	0
4	OLA	B	2017	18/20	0.81	0.11	79,98,112,114	0
4	OLA	A	2020	14/20	0.82	0.11	73,78,91,93	0
4	OLA	B	2013	16/20	0.83	0.16	109,114,120,121	0
4	OLA	A	2016	20/20	0.83	0.12	88,93,110,110	0
3	OLC	A	2002	9/25	0.83	0.11	80,81,84,84	0
3	OLC	B	2008	7/25	0.83	0.10	83,84,85,85	0
5	1PE	A	2021	10/16	0.83	0.11	111,112,114,114	0
4	OLA	A	2019	20/20	0.84	0.10	97,104,120,121	0
4	OLA	A	2014	7/20	0.85	0.13	92,96,105,108	0
4	OLA	A	2013	19/20	0.85	0.13	86,95,101,101	0
4	OLA	B	2012	10/20	0.86	0.10	87,96,105,105	0
3	OLC	B	2007	10/25	0.86	0.12	75,76,79,79	0
4	OLA	A	2012	8/20	0.86	0.14	85,88,98,100	0
3	OLC	B	2009	23/25	0.87	0.14	81,84,101,101	0
4	OLA	A	2011	13/20	0.87	0.11	102,112,120,121	0
4	OLA	B	2016	20/20	0.87	0.12	80,87,106,106	0
4	OLA	A	2015	7/20	0.87	0.12	76,83,94,94	0
4	OLA	B	2011	12/20	0.87	0.12	90,94,103,104	0
3	OLC	B	2005	10/25	0.87	0.11	90,95,97,97	0
3	OLC	B	2006	10/25	0.88	0.10	111,112,114,115	0
4	OLA	A	2018	6/20	0.88	0.11	69,70,72,72	0
3	OLC	A	2006	12/25	0.88	0.10	91,96,97,97	0
3	OLC	A	2008	9/25	0.88	0.12	75,78,81,81	0
3	OLC	B	2004	10/25	0.89	0.11	87,89,91,91	0
3	OLC	A	2007	16/25	0.89	0.12	84,96,118,119	0
3	OLC	B	2003	9/25	0.90	0.11	95,95,97,97	0
3	OLC	A	2009	7/25	0.90	0.11	70,71,78,80	0
3	OLC	A	2004	11/25	0.90	0.11	55,63,74,74	0
4	OLA	B	2014	9/20	0.92	0.08	87,90,96,97	0
2	ZLK	B	2019	41/41	0.92	0.11	53,63,72,77	41

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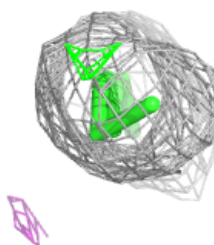
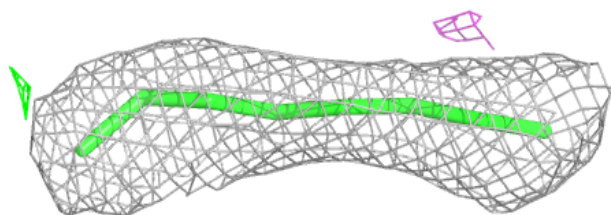
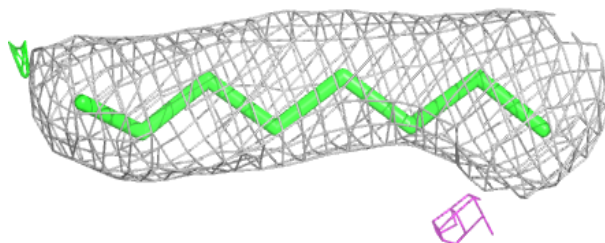
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OLC	A	2005	8/25	0.93	0.07	77,77,78,78	0
2	ZLK	A	2001	41/41	0.96	0.07	41,55,65,69	0
2	ZLK	B	2001	41/41	0.97	0.06	48,56,61,63	0
6	NA	A	2022	1/1	0.98	0.05	54,54,54,54	0
6	NA	B	2020	1/1	0.98	0.03	53,53,53,53	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

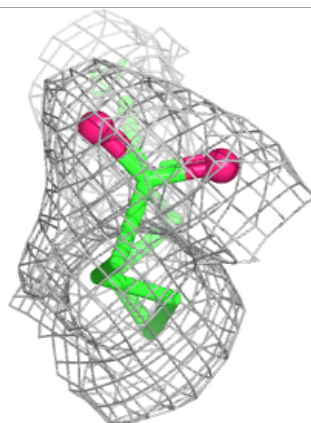
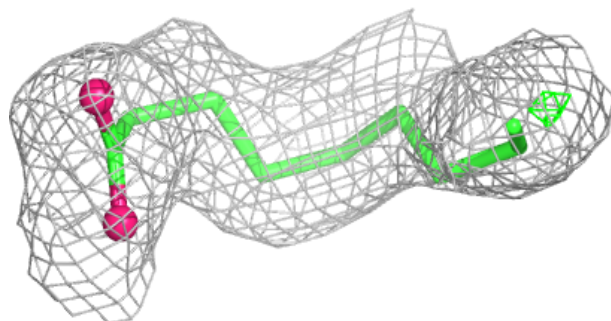
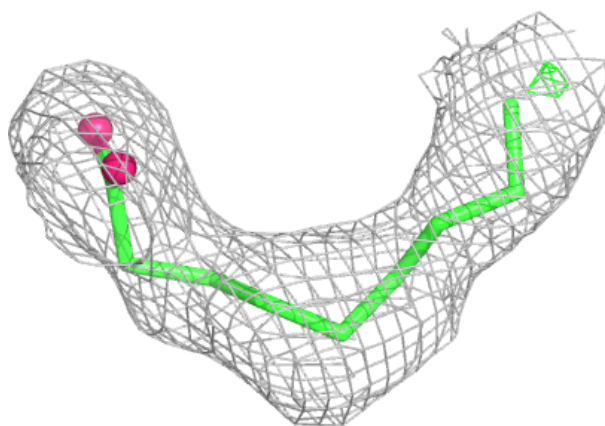


Electron density around OLC B 2002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

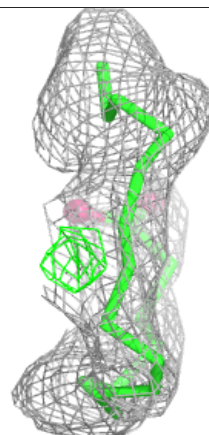
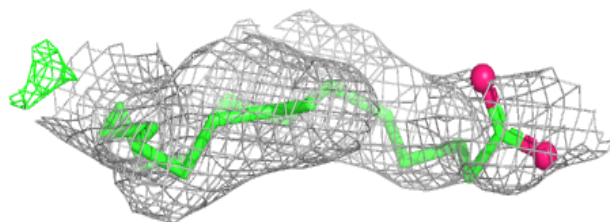
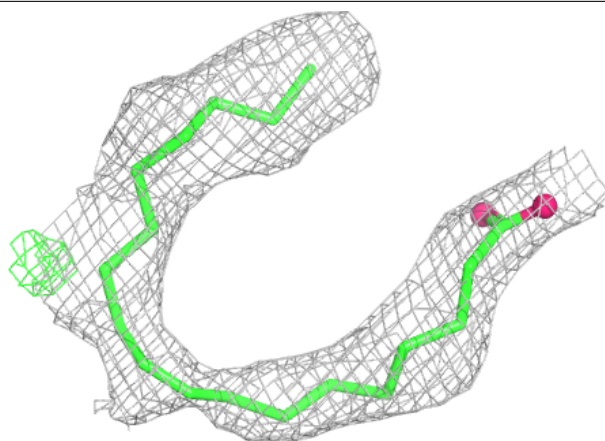
**Electron density around OLA A 2010:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



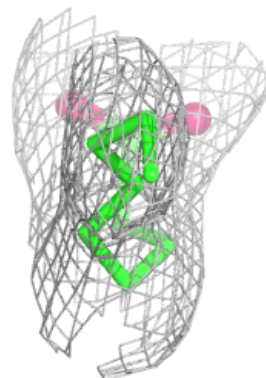
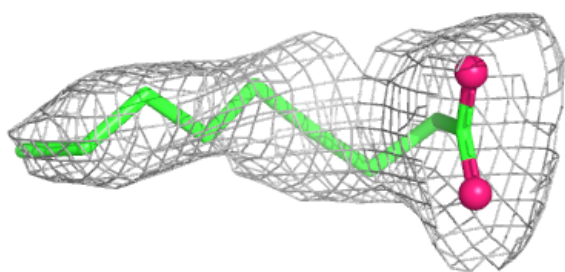
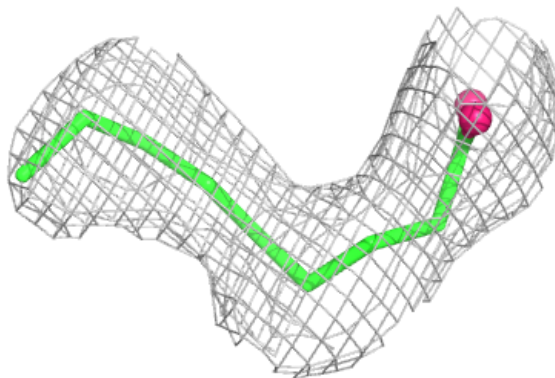
Electron density around OLA B 2018:

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and green (positive)

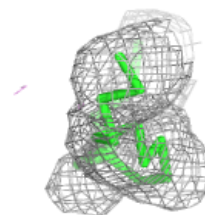
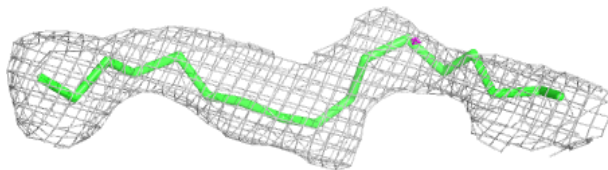
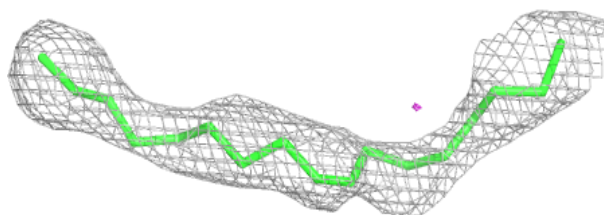


Electron density around OLA B 2015:

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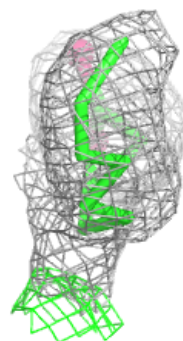
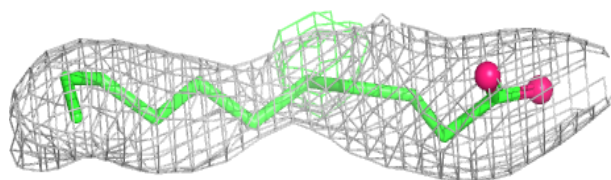
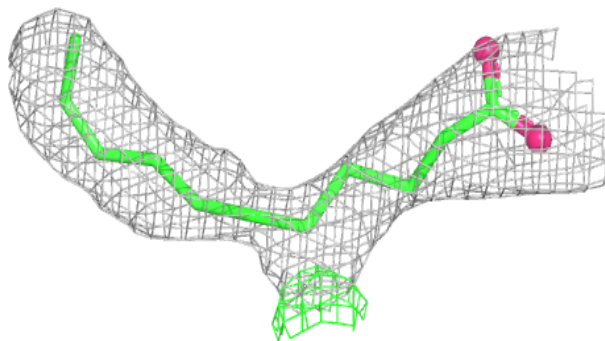
**Electron density around OLC A 2003:**

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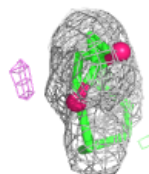
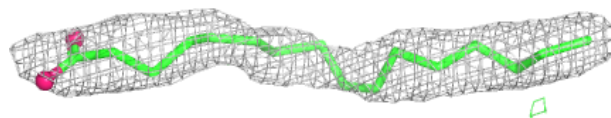
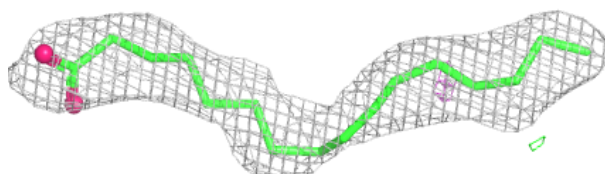


Electron density around OLA A 2017:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

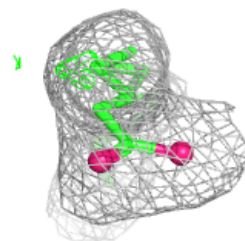
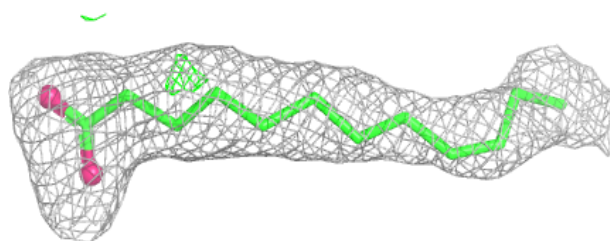
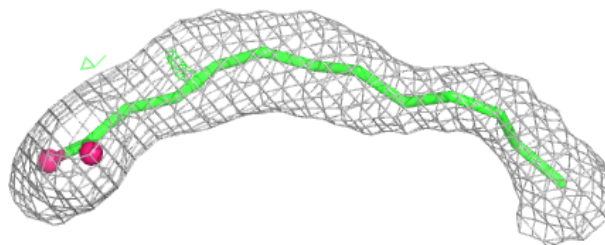
**Electron density around OLA B 2017:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

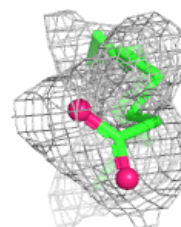
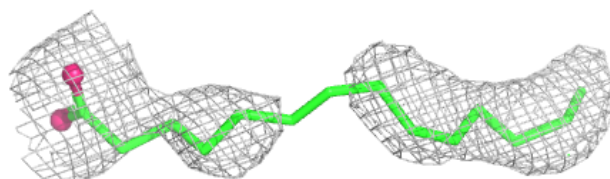
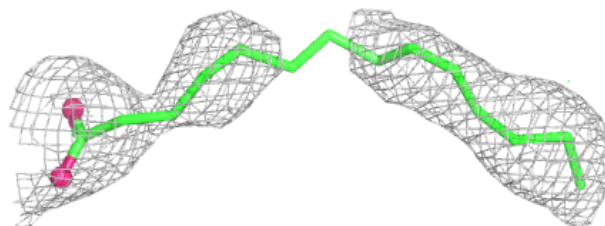


Electron density around OLA A 2020:

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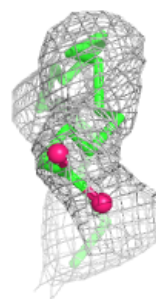
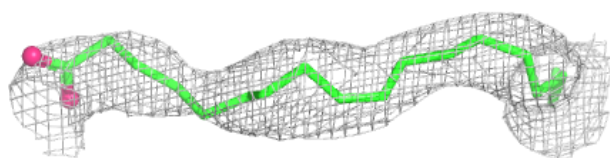
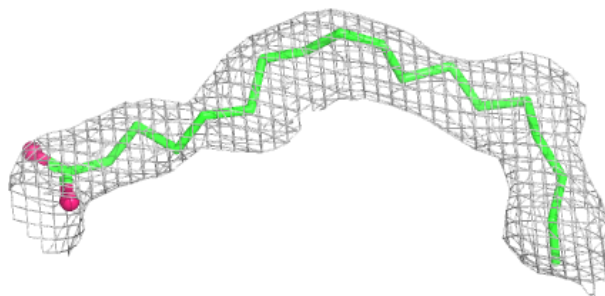
**Electron density around OLA B 2013:**

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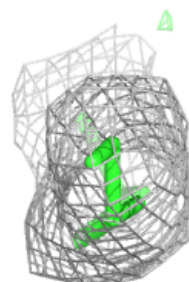
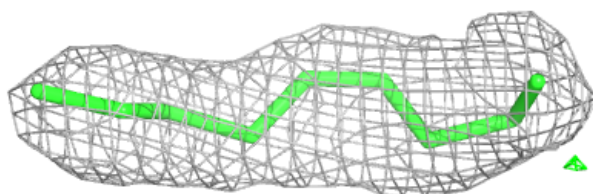
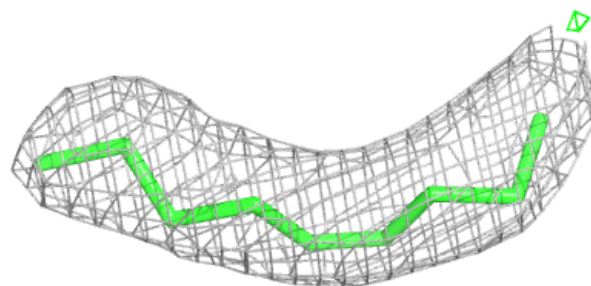


Electron density around OLA A 2016:

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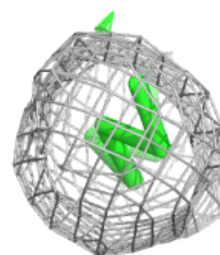
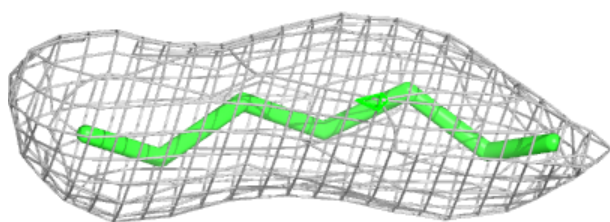
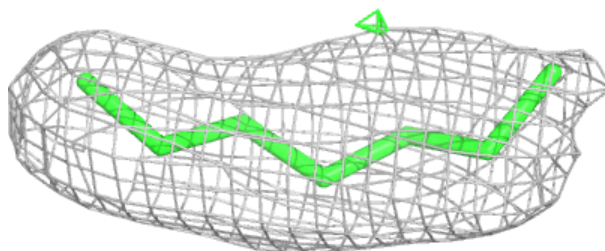
**Electron density around OLC A 2002:**

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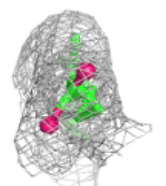
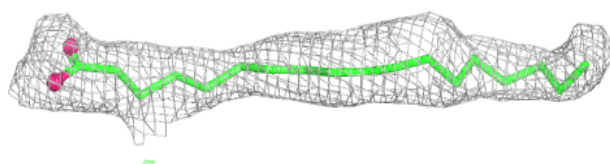
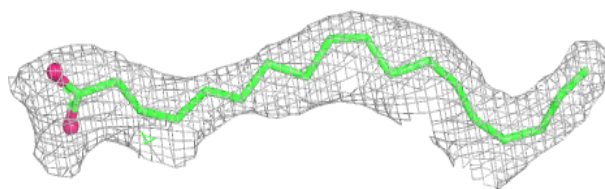


Electron density around OLC B 2008:

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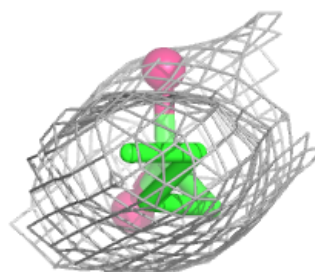
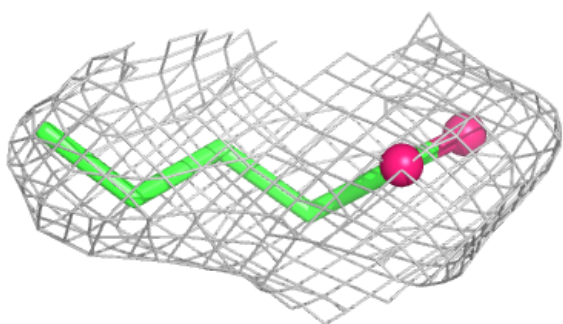
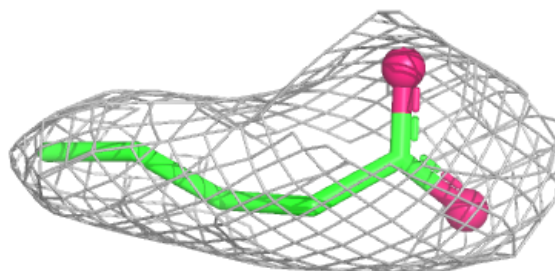
**Electron density around OLA A 2019:**

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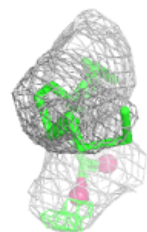
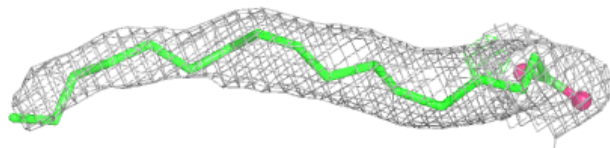
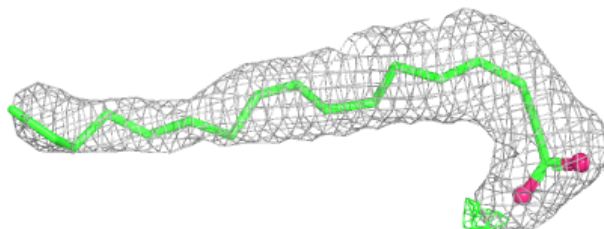


Electron density around OLA A 2014:

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and green (positive)

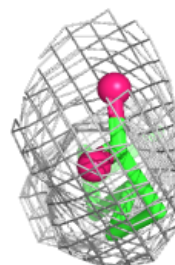
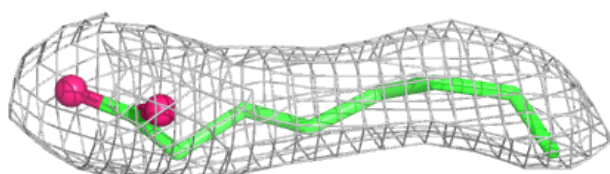
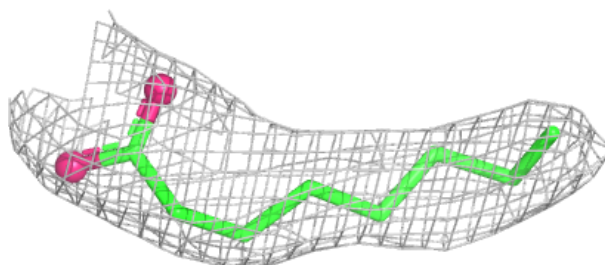
**Electron density around OLA A 2013:**

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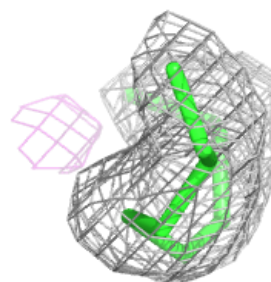
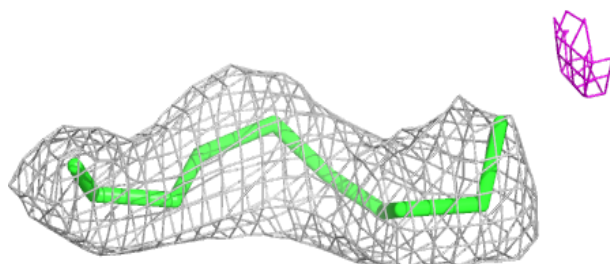
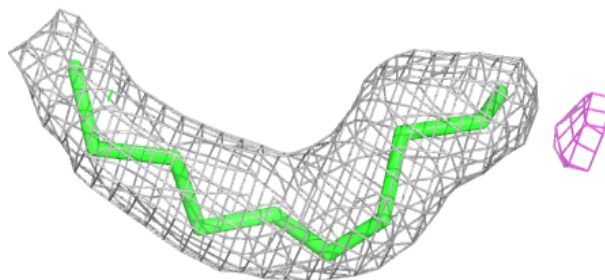


Electron density around OLA B 2012:

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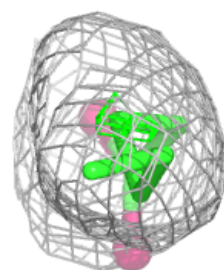
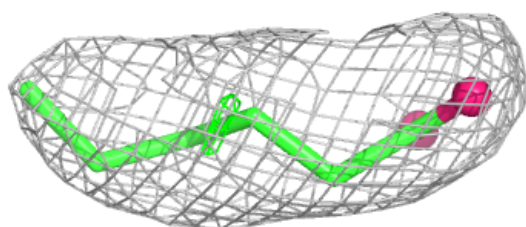
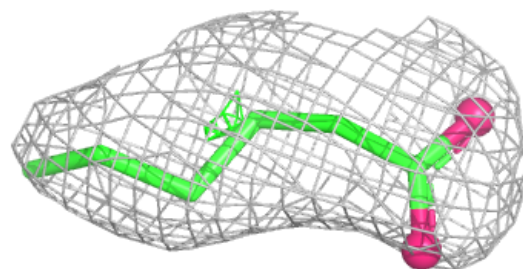
**Electron density around OLC B 2007:**

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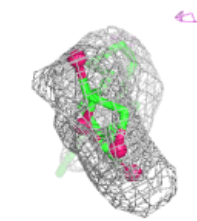
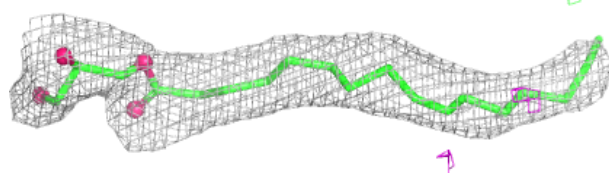
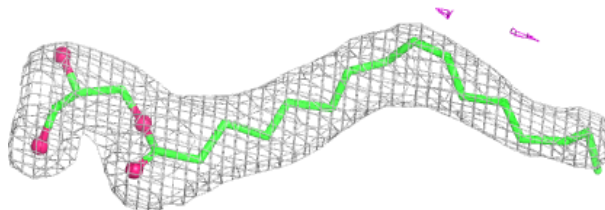


Electron density around OLA A 2012:

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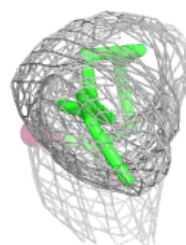
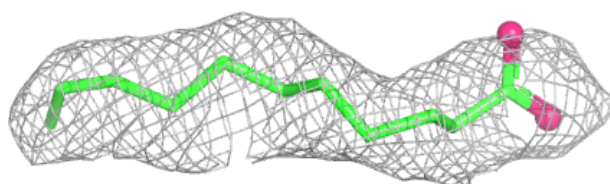
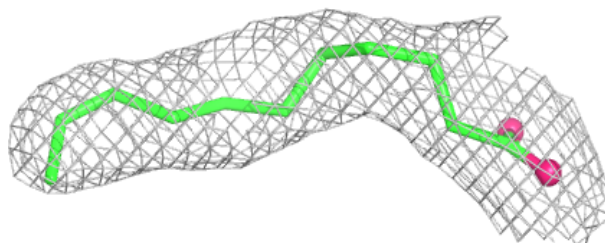
**Electron density around OLC B 2009:**

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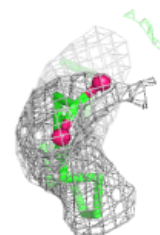
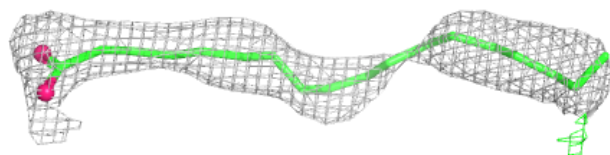
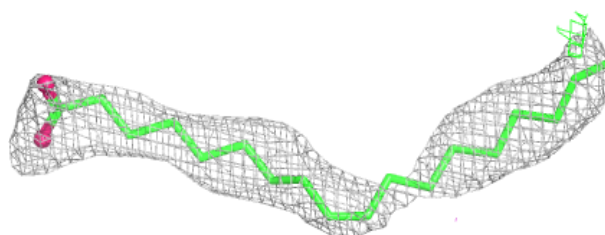


Electron density around OLA A 2011:

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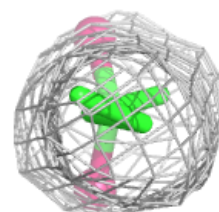
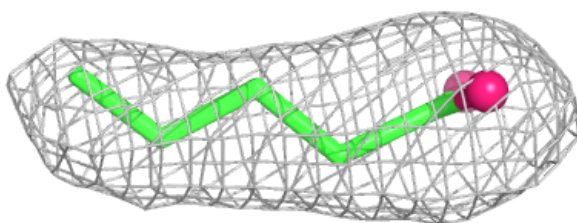
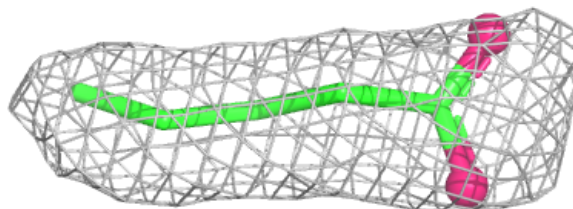
**Electron density around OLA B 2016:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

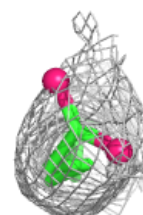
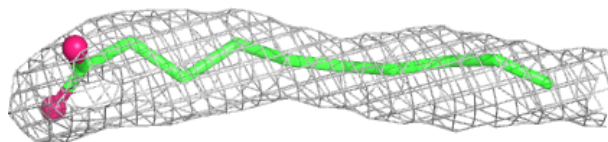
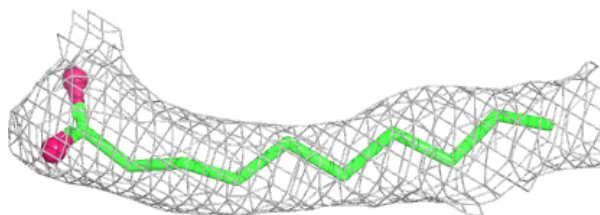


Electron density around OLA A 2015:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

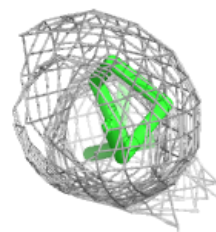
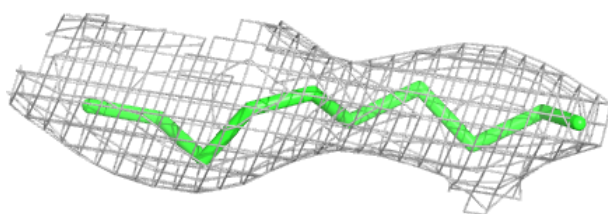
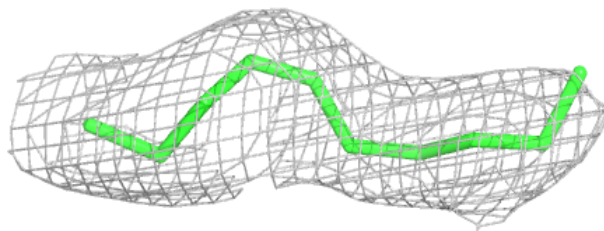
**Electron density around OLA B 2011:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

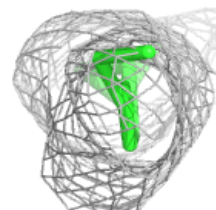
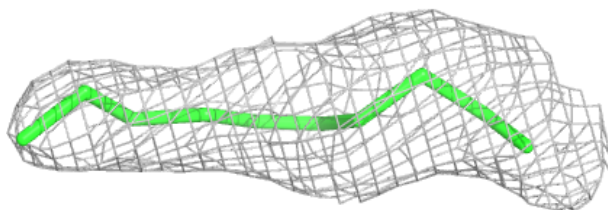
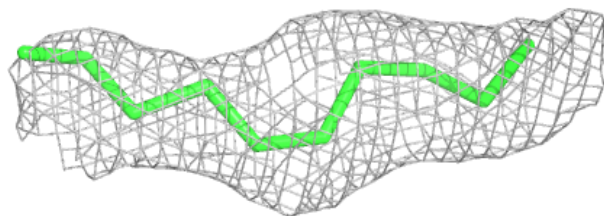


Electron density around OLC B 2005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

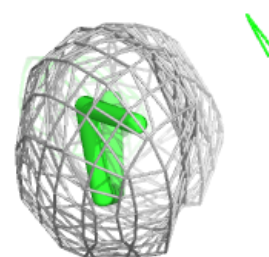
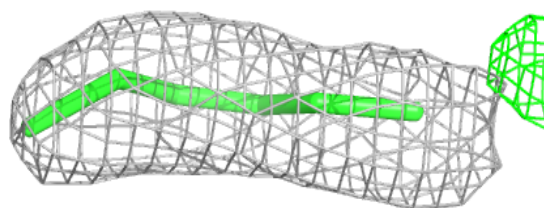
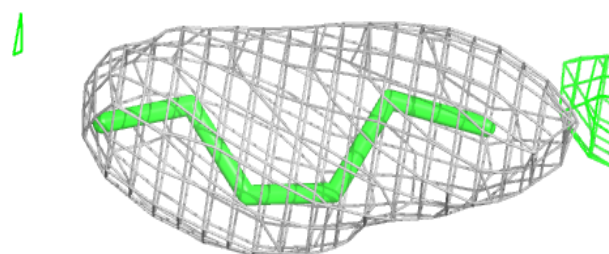
**Electron density around OLC B 2006:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

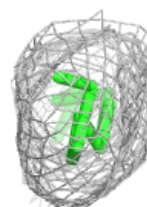
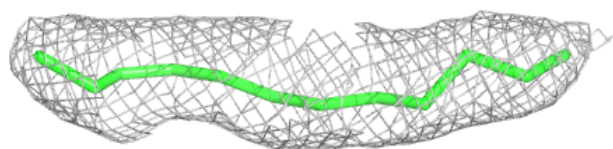
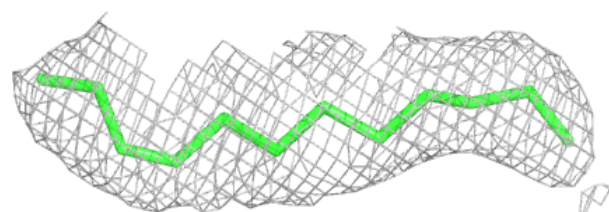


Electron density around OLA A 2018:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

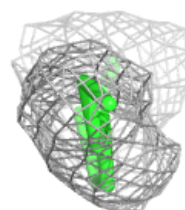
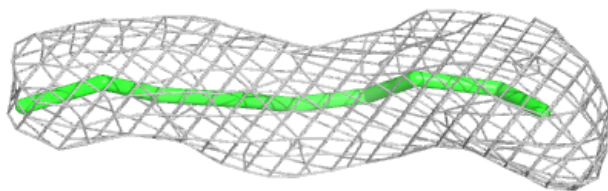
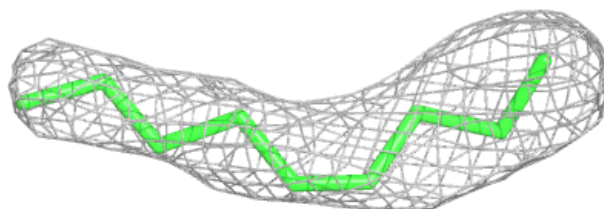
**Electron density around OLC A 2006:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



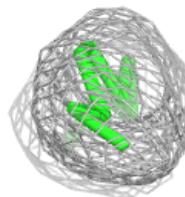
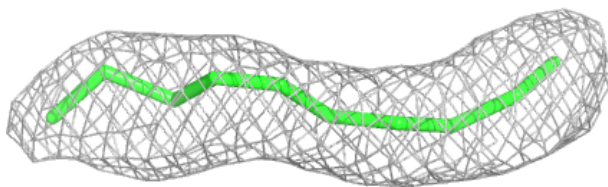
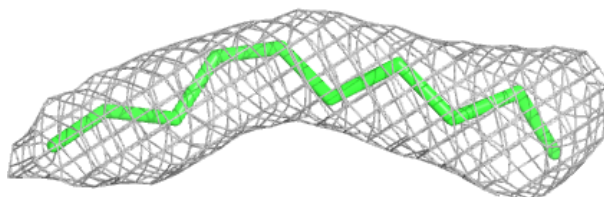
Electron density around OLC A 2008:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



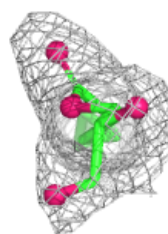
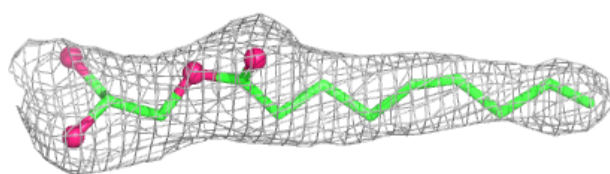
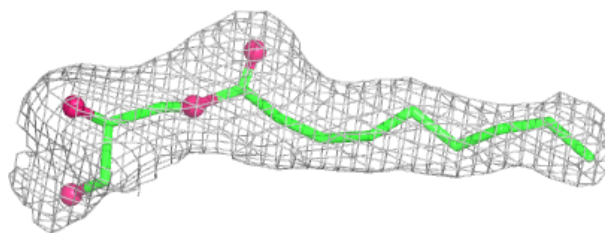
Electron density around OLC B 2004:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

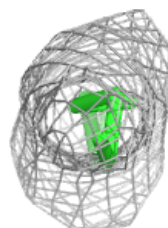
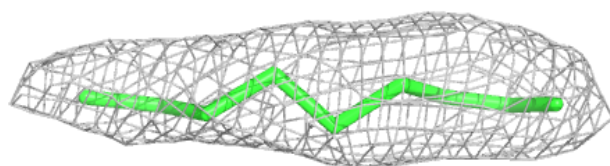
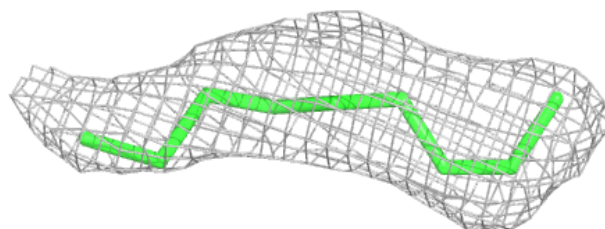


Electron density around OLC A 2007:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

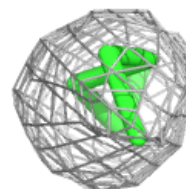
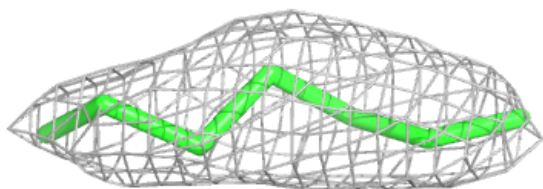
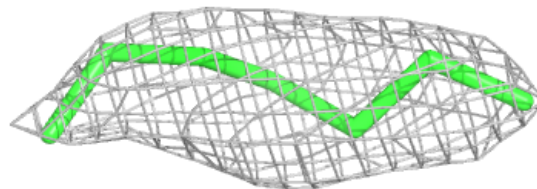
**Electron density around OLC B 2003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

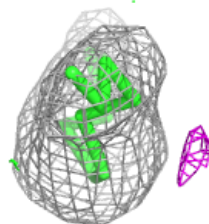
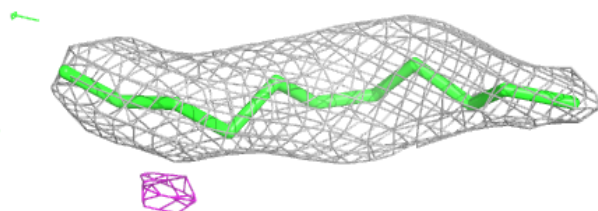
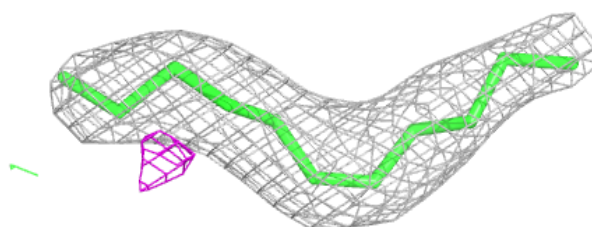


Electron density around OLC A 2009:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

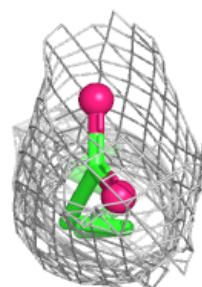
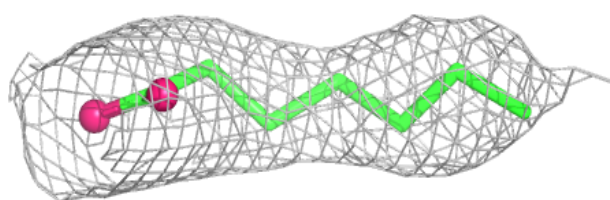
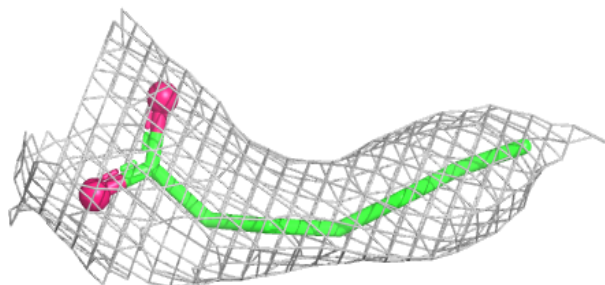
**Electron density around OLC A 2004:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

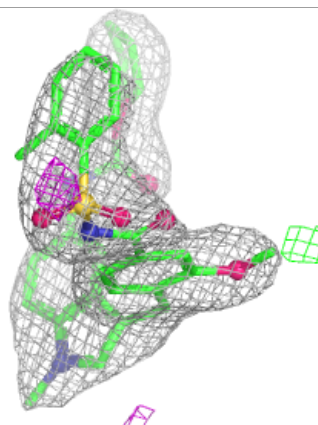
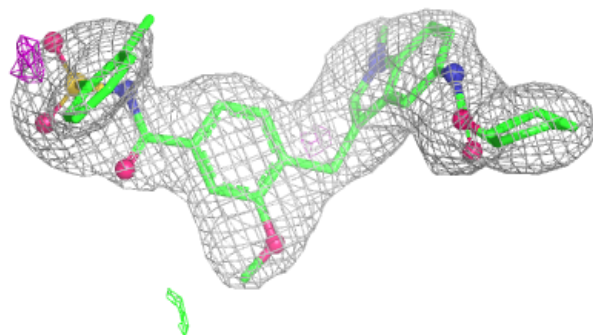
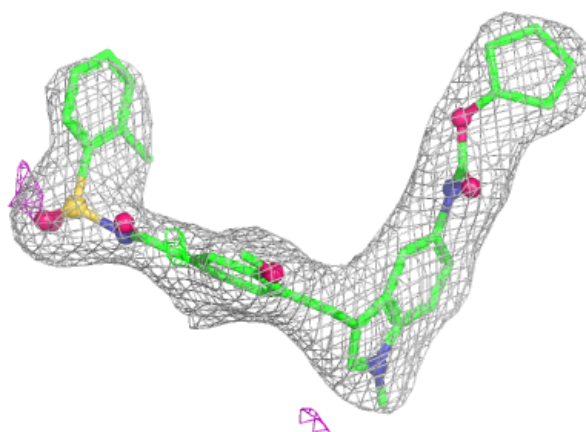


Electron density around OLA B 2014:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

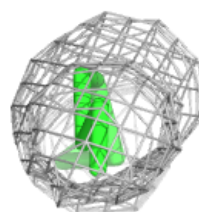
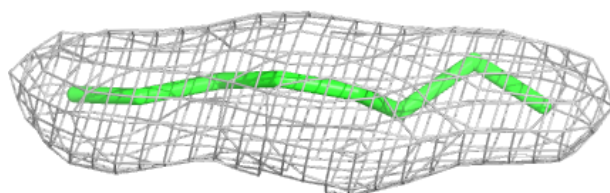
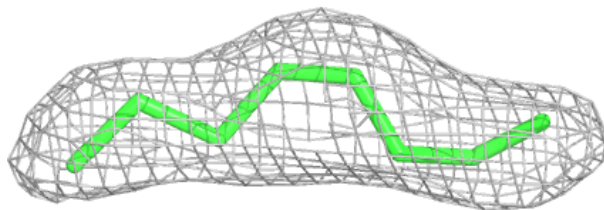
**Electron density around ZLK B 2019:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

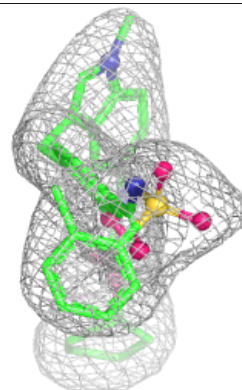
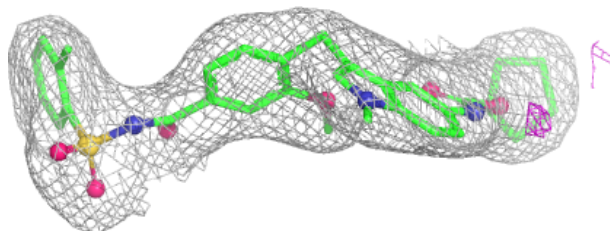
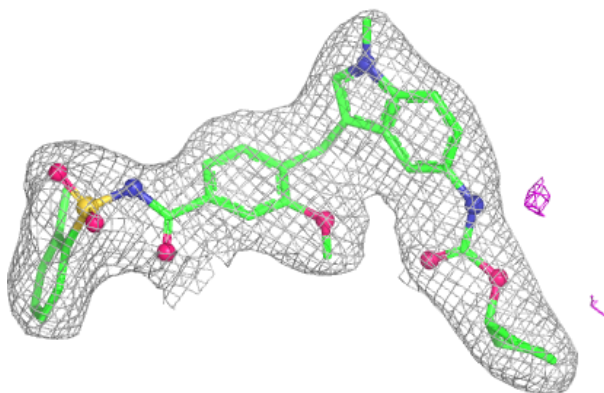


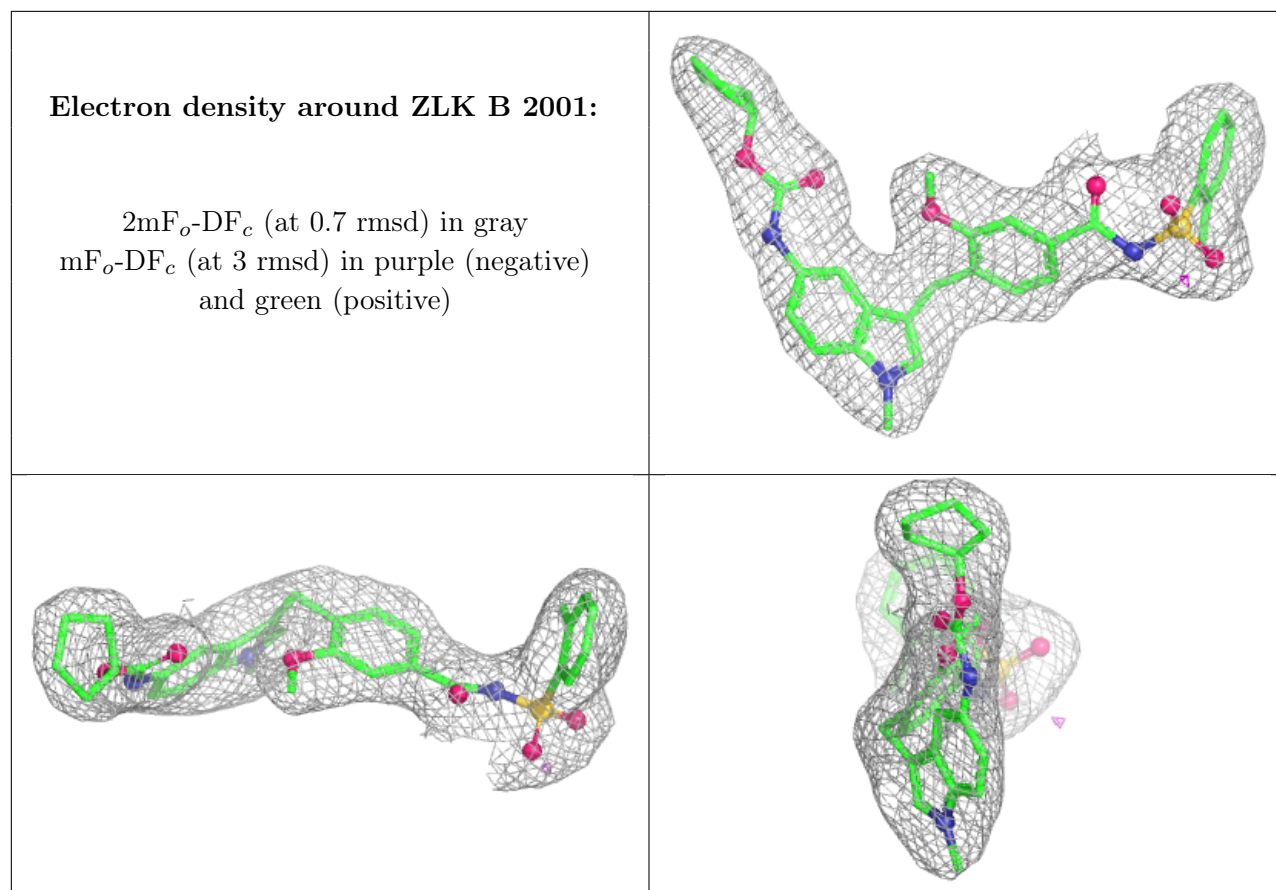
Electron density around OLC A 2005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ZLK A 2001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.